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Book of Abstracts

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MS04 / 1

A multiscale theory explaining the initial shrinkage of microporous materials upon adsorption

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Adsorption-induced deformation is widely observed in porous materials such as cement, coal, clay, aerogel, biopolymers, and MOFs. Sorption swelling has been commonly explained by the so-called Bangham effect (Bangham and Fakhoury 1928), i.e. the relaxation of solid-fluid interfacial tension due to adsorption and thus the macroscopic expansion of the porous media. However, experimental studies show that certain microporous materials (pore size less than 2 nm) such as activated carbons contract first at low gas pressure, followed by Bangham's expansion after reaching certain pressure levels (Balzer et al. 2015). Such phenomenon has not been explained and modelled in previous poromechanics theories.

This work extends the recently developed surface poromechanics framework for macro/meso porous media (Zhang 2018) to describe the adsorption-deformation behavior of microporous materials by considering interaction forces in micropores. At distances as small as a few nanometers, short-range intermolecular interactions can give rise to forces that are formerly disregarded in the analysis of macro/meso porous media. The effect of such interactions is considered in this study through an extra work term in the thermodynamics of a single slit pore. As a result of such pore-scale analysis, a pressure known as the disjoining or solvation pressure that acts normal to the pore walls in addition to the bulk fluid pressure is obtained. This effect also modifies the surface tension parallel to the pore walls. The disjoining pressure and the modified surface tension together create a competing effect in determining the shrinkage or expansion of the porous skeleton during adsorption. When the pore size becomes sufficiently large, this new development degenerates to the macro/meso poromechanics theory of Zhang (2018). Through a choice of adsorption and microstructure model, the proposed microporomechanics theory is validated against recent experimental data on activated carbons. To the author's knowledge, this is the first continuum theory that captures the initial shrinkage of microporous solids upon adsorption and is ready to be implemented in FEA or other numerical solvers for IBVP predictions.

Participation:

In-Person

References:

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Poster / 2

Permeability evolution of fractured sorptive porous materials

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Fractured sorptive geomaterials (FSG) are ubiquitous in geological systems such as coal, shale and chalk. The solid matrix of FSG can adsorb species in gas or liquid form, the process of which is often accompanied by the deformation and micro- structural alternation of the matrix. Such coupling is further obscured by the presence of fracture network, introducing complex fracture–matrix interactions. Predicting the hydromechanical properties of FSG is of particular importance for the production of coalbed methane (CBM) which requires the assessment of coal permeability under varying pressure and stress conditions. This study attempts to investigate the interplay between adsorption, deformation, and permeability evolution of coals. The novel concept of adsorption stress popularized in material science research is adopted here to construct a mechanistic theory describing sorption-induced deformation of coals. The constitutive theory is implemented in a finite element (FE) scheme and then adopted for describing coal matrix in a FE model of coal–fracture system. The model is calibrated for San Juan coals and applied to simulate a typical methane depletion test. It is observed that, depending on the competing effect between desorption-induced fracture opening and poroelastic compaction, the predicted permeability curve may be monotonically increasing (rising type) or decreasing (decline type), or may exhibit reduction first and then increase (rebound type) during gas depletion. Such competition is found to be controlled by the volume ratio, the permeability ratio, and the stiffness ratio between the matrix and the fracture elements. The prediction covers a wide range of permeability data obtained from laboratory tests and field observations.

Participation:

In-Person

References:

Zhou, X., Liu, S. and Zhang, Y., 2021. Permeability evolution of fractured sorptive geomaterials: a theoretical study on coalbed methane reservoir. Rock Mechanics and Rock Engineering, 54(7), pp.3507-3525.

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MS07 / 3

Multiscale modelling of plant nitrogen use efficiency

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Nitrogen fertilization is vital for productive agriculture and efficient land use. However, globally, approximately 50% of the nitrogen applied is lost to the environment, causing inefficiencies, pollution, and greenhouse gas emissions. Rainfall and its effect on soil moisture are the major components controlling nitrogen losses in agriculture. Thus, changing rainfall patterns could accelerate nitrogen inefficiencies. We first used the pore scale model from XCT to assess the effect of single fertiliser granule dissolution on soil pore scale N dissolution and microbial processes. Then we upscaled this model to the field scale and used a mechanistic modeling platform to determine how this influences field scale processes. Following this we used the plant N uptake model to determine how precipitation-optimal nitrogen fertilization timings and resulting crop nitrogen uptake have changed historically (1950–2020) and how they are predicted to change under the RCP8.5 climate scenario (2021–2069) in the South East of England. We found that that the interannual variation in precipitation-optimal uptake is projected to increase. Ultimately, projected changes in precipitation patterns will affect nitrogen uptake and precipitation-optimal fertilization timings. We argue that the use of bespoke fertilization timings in each year can help recuperate the reduced N uptake due to changing precipitation.

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Poster / 6

Quantitative characterization of pore structure and analysis of seepage characteristics of tight reservoir based on digital core and NMR

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Quantitative characterization of pore structure and analysis of seepage characteristics of tight reservoir based on digital core and NMR
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Abstract: The pore-fracture structure characterization and seepage characteristics analysis are the keys to the effective development of tight reservoirs. However, it is difficult to accurately characterize the pore and fracture structures of different scales by conventional methods, which makes it

difficult to analyze the seepage characteristics. In this study, combined with CT scanning technology and advanced mathematical algorithms of AVIZO visualization software, a three-dimensional digital core of tight reservoirs was constructed, and the comprehensively quantitative characterization of microscopic pore-fracture structure from multiple dimensions was carried out. On this basis, nuclear magnetic resonance (NMR) centrifugation experiments were conducted to monitor the fluid migration dynamics in tight reservoirs, and mobile fluid migration characteristics were analyzed based on NMR T2 spectra. The results show that the average porosity of the reservoir in this area was 11.2%, and the average permeability was 1.573mD, which belongs to low porosity and low permeability tight reservoirs. The distribution of pore throats was mainly contiguous and isolated. The connected pores were mainly distributed in enriched bands, which was due to the interconnection of gas pores, intergranular pores, and dissolution sheet fractures, while the disconnected pores were mainly distributed in isolated form, which was related to the development of inter-gravel dissolved pores and matrix dissolved pores, and the contribution of pore connectivity to seepage was greater than that of pore scale. The pore radius in this area was mainly 4.31-32.17 μm, the throat radius was mainly 3.42-13.29 μm, and the pore and throat cross-sectional shapes were mostly triangular, meanwhile, the fracture types could be divided into 3 types according to the occurrence and opening, which were mainly high-angle structural fractures and vertical fractures, indicating that pore-fracture structure had strong heterogeneity and fractures could play a better role in the infiltration of oil and gas. The connectivity of pore throats in the tight matrix was poor, which made the imbibition exchange effect weak and prone to water sensitivity. Subsequently, the movable fluid saturation increases with the increase of permeability, and the fractures and micropores had less flow resistance and were more conducive to water flow compared with small pores. This case study provides new insights into the exploitation of similar tight reservoirs.
Key works: NMR; dual porous medium; CT scanning; cross scale; digital core; quantitative characterization of pores fractures; fluid mobility

Participation:

In-Person

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Poster / **7**

Investigation of reaction rates during microbiologically induced calcium carbonate precipitation

Author: Niklas Erdmann[1]

Co-authors: Susanne Schaefer [2]; Ulrich Bröckel [2]; Dorina Strieth [1]

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[2] *Trier University of Applied Sciences, Department of Environmental Planning and Technology, Environmental Campus Birkenfeld*

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With a share of about 8.6 % of anthropogenic CO2 emissions, concrete is a major contributor to global warming. Microbiologically induced calcium carbonate precipitation (MICP) offers the potential of a more sustainable alternative. During MICP calcium carbonate is formed by microbiological activity and can serve as a binder between mineral particles. This calcium carbonate can be an alternative binder to conventional cement mortar used for concrete. The most commonly used mechanism for MICP is ureolysis. In this process, urea is enzymatically degraded to ammonium and carbonate. In the presence of calcium ions and in an alkaline environment, calcium carbonate precipitates. Since the compressive strength after MICP is related to the amount of precipitated calcium carbonate, multiple cycles of treatment with cell suspension and calcination solution are necessary if high compressive strengths need to be achieved. It is therefore of interest to improve treatment times by obtaining knowledge of the reaction speed of ureolysis. Various studies have investigated the rate and kinetics of MICP regarding the concentration of cells, urea and calcium ions. However, only low concentrations of calcium ions (up to 500 mM) and cells (up to OD600 1) have been investigated so far. In order to obtain insight into the efficiency of MICP under conditions during the production of biocement, this study investigated MICP for calcium and urea concentrations up to 1391 and 1492 mM, and cell concentrations with an OD600 up to 10. It was shown that the rate of MICP continuously decreases with the addition of calcium ions. Furthermore, it could be observed that under these conditions the free calcium ions are degraded by formation of calcium carbonate within a few hours. During this time Sporosarcina pasteurii cells encapsulate in calcium carbonate while still maintaining ureolytic activity. Depending on the parameters reaction times under 3 hours were achieved which is significantly shorter than the reaction time of 24 hours often used in literature protocols for MICP treatment. Therefore, these findings make it possible to determine an optimum reaction time for the production of biocement depending on the cell concentration and the composition of the calcination solution used during MICP. Based on these results silica sands with different particle size distributions were treated with several injection methods under these optimised conditions. The resulting samples were scanned by micro computed tomography. Contact points and pore space depending on various parameters during the treatment of MICP were investigated. These findings can be used to further investigate if a reduced reaction time between cycles is applicable concerning compressive strength and homogeneity of the samples.

Participation:

In-Person

References:

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MS07 / **8**

The Darcy-type boundary condition on a porous wall

Authors: Igor Pažanin[1]; Eduard Marušić-Paloka[1]

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The aim of this talk is to present the derivation of the new effective boundary condition for the fluid flow in a domain with porous boundary. We start from the Stokes system in a domain with an array of small holes on the boundary and on each hole we impose an appropriate dynamic condition, namely the value of the normal stress corresponding to the exterior conditions. The goal is to obtain the effective model by studying the convergence of the homogenization procedure, as the period of the porous boundary tends to zero. As a result of our analysis, we propose the interface condition in the form of the generalized Darcy law. If no further assumptions are made concerning the isotropy of the geometry of the porous boundary, the obtained result generalizes the Beavers-Joseph condition. In the second part of the talk, we shall also study the roughness-induced effects on the proposed Darcy-type boundary condition.

Participation:

In-Person

References:

E. Marušić-Paloka, I. Pažanin, The effective boundary condition on a porous wall, International Journal of Engineering Science 173 (2022), 103638, pp. 1-12.

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10

APPLICATION OF SUPER-RESOLUTION CONVOLUTIONAL NEURAL NETWORK TO IMPROVE THE RESOLUTION OF DIGITAL ROCK MICRO-CT IMAGES

Authors: Ramin Soltanmohammadi[1]; Shohreh Iraji[1]; Joao Paulo da Ponte Souza[1]; Mateus Basso[1]; Alexandre Campane Vidal[1]

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High-quality digital rock images are crucial to precisely assess the petrophysical characteristics as well as flow properties in pore-scale porous media. However, the captured-image quality is governed by the limitations of the detectors' and scanners' hardware. The pore network model, multi-mineral segmentation, permeability prediction, and flow streamlines modeling in the porous material can all be significantly impacted by the scanner constraint. It is notably noticeable in carbonate rocks, where up to 50% of the pores may have a diameter smaller than the resolution of a micro-computed tomography (micro-CT) scanner [4]. To address this issue, we utilized a convolutional neural network-based model, trained on a massive dataset of images, to improve the resolution of micro-CT images. The super-resolution convolutional neural network (SRCNN) method is a feed-forward convolutional neural network (CNN) with three 2D-convolutional layers with kernel sizes of 9, 1, and 5, as well as 64, 32, and 3 filters, respectively [1]. SRCNN is used to construct a super-resolution (SR)

image from a single low-resolution (LR) image, which is downsampled and blurred, and generated via bicubic interpolation. The parametric rectified linear unit (PReLU) activation function was utilized for the first two layers, and the linear activation function was used in the final layer. The objective loss function (mean squared error) was optimized to determine the weights and biases of layers using the Adam optimizer. The size of the LR images produced by bicubic interpolation, the generated SR, and the micro-CT images (HR) are all $128 \times 128 \times 3$ pixels, and the SRCNN model had a total of slightly more than 1.5 million parameters.
The SRCNN method was trained on a dataset containing over 20,000 micro-CT images collected from Brazilian Stromatolite plug samples in order to boost image resolution and capture the pore space geometry in more detail. We allocated 20% of the data (about 4,000 micro-CT images) to the test set and the remaining data to the training set. The stromatolite outcrop samples utilized in this research were taken from Lagoa Salgada in Rio de Janeiro, Brazil, and were scanned using a ZEISS XRadia-Versa XRM-500 micro-CT scanner with $40 \frac{\mu m}{voxel}$ spatial resolution.
Two metrics are used to evaluate image reconstruction quality: peak signal-to-noise ratio (PSNR) and structural similarity index measure (SSIM) [2,3]. The comparison of LR and generated SR images with HR data ascertained a notable boost in the resolution, where PSNR rose from 76.95 dB to 79.87 dB and SSIM increased from 0.89 to 0.92. The results demonstrated that noisy, blurry LR images could be converted into high-fidelity SR images by using the SRCNN architecture. The edge and boundary features, which are critical for pore-scale modeling, were successfully captured in the generated SR images. In addition, we were successful in recreating the intricate texture of the micro-CT images with the use of a relatively shallow CNN model. The trained model was then implemented in the original micro-CT scans, resulting in the production of more elaborated digital rock images.

Participation:

Online

References:

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Poster / 15

Atomistic Insight into Trapped Oil Displacement by Nanofluids

Author: YUANHAO CHANG[1]

Co-authors: Zhiliang Zhang [1]; SENBO XIAO [1]; JIANYING HE [1]

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Nanofluids possess great application potential in enhanced oil recovery (EOR). However, the EOR effects and mechanisms of nanofluids with specific nanoparticles (NPs) are not clear. In the study, the molecular dynamics (MD) simulation is thus adopted to explore the displacement of trapped oil in the rough channel by various nanofluids. Our results indicate that nanofluids with hydrophilic NPs and Janus NPs hold a greater EOR effect (9.7% and 7.1%, respectively), while hydrophobic ones are not suitable for oil film (with EOR effect of 2.3%). Specifically, hydrophilic NPs increase the viscosity and the sweeping scope of injected fluid. Janus NPs are prone to stay at the oil-water interface to reduce the interfacial tension. Most of them adsorb on the bulge, alter the surface wettability, and squeeze the trapped oil while others remobilize the trapped oil by sliding along the interface. Due to the entering of a large number of hydrophobic NPs inside the oil clusters, the influence of oil molecules being bound by NPs greatly reduces the effect of volume replacement, which leads to a poor displacement effect and even a risk of plugging the channel. Among the nanofluids, the ones with Janus NPs can maintain a stable oil displacement performance under low pumping force, thanks to sufficiently long contact time between Janus NPs and the oil phase. Further analysis on capillary number highlights the applied prospect of Janus NPs in actual oil reservoirs. Our findings are favorable to understanding the mechanism of nanofluids in EOR and provide guidance on the screen of NPs.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 16

Perturbation Theory and Green's Function to Solve the Non-Linear Dispersion Saturation Equation arising in Cyclic Injection-Production Well Tests

Authors: Cintia Goncalves Machado[1]; Albert Reynolds[2]

[1] *TNO*

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Well testing is a common practice that consists of wellbore pressure and flow rates data acquisition in order to estimate parameters that govern multiphase flow in a porous media. An injection-falloff-production test was originally proposed by Shi et al (2006) as a well test for the in-situ estimation of

two-phase relative permeability curves. The idea is based on the concept that if a well is returned to production subsequent to an injection-falloff test, then during the production period, the sandface will be exposed to a range of saturations. Consequently, the wellbore pressure during the flowback period is influenced by the changing saturation in the near wellbore region and hence contain information about the two-phase relative permeability curves. Although the wellbore pressure during injection and falloff seems to be insensitive to the dispersive effects of capillarity, knowledge of the correct saturation profile at the end of injection represents the initial condition for the falloff period, and is required to calculate the saturation distribution during falloff. The saturation distribution at the end of the falloff is required as the initial condition for the production period. In previous work we applied the method of matched asymptotic expansions to solve the one-dimensional saturation convection-dispersion equation, a non-linear pseudo-parabolic partial differential equation. This equation is one of the governing equations for two-phase flow in a porous media when including capillary pressure effects, for the specific initial and boundary conditions arising when injecting in an infinite radial piecewise homogeneous horizontal medium. If the total flow rate becomes equal to zero as in a falloff test, the saturation convection-dispersion equation reduces to a non-linear parabolic equation, which contains only a dispersion (diffusion) term. In this work, we find a closed form solution for the saturation distribution by applying the perturbation theory together with a Green‘s function, treating the non-linearity as a source term. By combining the solution for saturation with the so-called Thompson-Reynolds steady-theory method for obtaining the pressure, one can obtain an approximate analytical solution for the wellbore pressure, which can be used as the forward solution to analyzing pressure data by pressure transient analysis.

Participation:

In-Person

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MS09 / 17

A Lubrication Model for Wettablity Characterization

Author: Mojtaba Norouzisadeh[1]

Co-authors: Philippe Leroy [2]; Mohamed Azaroual [3]; Cyprien Soulaine [1]

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Trapping of fluid in porous media by capillary forces is a key process in many subsurface processes. It can be favorable to store carbon dioxide in deep saline aquifers, or unfavorable for groundwater remediation and in petroleum production, where droplets of contaminants/oils are trapped in the pore-space by capillary forces. Wettability properties at the vicinity of three-phase contact region is a key parameter to describe trapping mechanisms as well as the long-term stability of trapped droplets. Although the concept of contact angle –i.e. the angle visually measured between the solid

surface and the fluid-fluid interface –is widely used to model two-phase flow processes at the pore-scale, it does not accurately describe wettability alteration due to change in pH and salinity. The latter arises from inter-molecular interactions. Furthermore, the variation of contact angle with the velocity field at the three-phase contact region gives rise to more complications. This region is created by spreading of a thin film of one phase on the solid as oppose to the other fluid and is thin enough to be in the range of inter-molecular forces. We intend to model the wettability by investigating the evolution of this film.

To do so, we developed a lubrication model for the thin film evolution on the solid surface. The model is physically rooted and replaces the concept of contact angle. It accounts for inter-molecular forces by introducing the different components of the disjoining pressure, notably the van der Waals and electric double layer potentials. The developed framework relates molecular interactions to pore-scale simulations through the boundary conditions, paving the way to more realistic pore-scale simulations with wettability alterations. It also can be used as a tool to investigate other phenomena governed by inter-molecular forces, such as film stability and streaming potential.

For the particular case when the film contains electrolytes, the different ions will get adsorbed on the solid surface. Even though the fluid charge is neutral, a distribution of ions will form close to the solid surfaces. Movement of fluid in this region will create an electrical voltage called streaming potential. The effect of streaming potential can be noticeable, especially in the case of moving contact line. We would like to study the movement of the ions in this region in order to find out the range of the importance of streaming potential.

Participation:

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MS09 / 18

Dispersion of a passive scalar around a confined bubble

Authors: Davide Picchi[1]; Pietro Poesio[2]

[1] *Università degli Studi di Brescia*

[2] *University of Brescia*

Corresponding Authors: pietro.poesio@unibs.it, davide.picchi@unibs.it

The study of mass-transfer in confined geometries is extremely important in many engineering and biological systems. In the context of geological carbon sequestration, carbon dioxide is injected into subsurface reservoirs leading to the formation of elongated bubbles that can either be trapped, move, or interact with the solid matrix. The presence of carbon dioxide has the effect of increasing the acidity of the in-situ brine, boosting a series of chain reactions that enhance rock dissolution. This may threaten the long-term integrity of the storage process due to the formation of leakage pathways for carbon dioxide.

Although the hydrodynamics of elongated bubble has been object of several studies, the case where a solute is transported in the surrounding liquid and surface mass-transfer mechanisms act on the solid wall or the bubble-fluid interface is much less understood. To fill this gap, we investigate the transport problem around a confined Taylor bubble to access the competition between advection, diffusion, and surface mass-transfer in the different regions of the bubble. To this aim, we derive a one dimensional Advection-Diffusion-Mass-Transfer equation where the transport mechanisms are described through an effective velocity, an effective diffusion coefficient, and an effective Sherwood number. Our model generalises the Aris-Taylor dispersion to the case of a Taylor bubble and clarifies the impact of surface mass-transfer in the advection and diffusion dominated regimes for both the front and rear menisci.

Despite the fact that the motivation of our work is oriented to microfluidics applications that involves solute transport and mass-transfer, its ramifications are relevant also in scenarios where the presence of a solute affects the surface tension (i.e., Maragoni effect) or even drives the flow (i.e., diffusioosmosis).

Participation:

In-Person

References:

Picchi, D., & Poesio, P. (2022). Dispersion of a passive scalar around a Taylor bubble. Journal of Fluid Mechanics, 951, A22. doi:10.1017/jfm.2022.829

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Poster / 19

Transport and evaporation of aqueous co-solvent solutions in thin porous media

Authors: Mirjam G. Wijburg[1]; Shuo Wang[1]; Anton Darhuber[1]

[1] *Eindhoven University of Technology*

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We have studied the imbibition and drying of water/co-solvent mixtures in paper and glass microfiber filters. The experiments reveal a rich interplay of solution imbibition, solvent evaporation and solvent-mediated pore-fiber transport. After deposition, liquids occupy the micron-scale inter-fiber pores of a paper sheet. In thermodynamic equilibrium, polar liquids such as water and co-solvents reside in the nm-scale intra-fiber pores of the cellulose fibers. The timescales for attaining equilibrium prove to depend sensitively on the water content, such that co-solvents can be temporarily trapped in a non-equilibrium configuration. The combination of two experimental methods allows the determination of both the overall co-solvent content and an estimation of what fractions reside in the pores and in the fibers of a paper sheet. The results are relevant to understanding the behavior of solutions in paper and provide insight into the dynamics of aqueous inkjet printing inks.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 20

Transient deformation and swelling of paper by aqueous co-solvent solutions

Authors: Chee-Lok Wong[1]; Shuo Wang[1]; Sajjad Karimnejad[1]; Mirjam G. Wijburg[1]; Hamid Mansouri[2]; Anton A. Darhuber[1]

[1] *Eindhoven University of Technology*

[2] *Canon Production Printing*

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Inkjet printing inks frequently contain polar liquids of low volatility such as glycerol or poly(ethylene glycols) in addition to water as the main solvent. The deposition of these liquids on paper sheets induces swelling of the cellulose fibers, which leads to an overall, anisotropic deformation of the sheet. We characterized the corresponding strain components by means of a grid projection method and white light interferometry. For pure water, most of the hydroexpansion strain vanishes again after drying is complete. However, for aqueous solutions of non-volatile co-solvents, a large fraction of the deformation persists after the water has evaporated. Because swelling occurs only after liquid enters the cellulose fibers, monitoring the dynamics of expansion provides insight into the pore-fiber distribution of co-solvents. The corresponding timescales of pore-fiber transport strongly depend on the co-solvent concentration, as a sufficient quantity of water is needed to plasticize the fiber walls.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS22 / 22

Noble metal coated high-aspect-ratio nanopore arrays and porous nanotube networks for catalysis in chemical synthesis and fuel cells

Author: Wolfgang J. Ensinger[1]

Co-author: Manfred E. Ensinger [1]

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Nanopore arrays, fabricated by the track-etching technique, mostly in Polycarbonate (PC) or Polyethylenterephthalate (PET) foils, are commercially available. These are formed by irradiation with highly energetic ions, such as Ar, from e.g. a cyclotron, and chemically etching the damage tracks up into cylindrical nanopores. For the present study, a linear heavy ion accelerator was applied, and, next to PC and PET, also Polyimide with a better chemical and thermal stability than the polyesters was used. The foils were up to 30 µm thick, the nanopores with an areal density up to 10-9 cm-2 had a diameter of down to 10 nm, corresponding to very high aspect ratio tubes.
Uniformly coating the inner walls of those nanopores with a thin reactive metal film constitutes a challenging process, since the thin film material transport into the nanopores has to be well controlled, particularly to avoid clogging of the apertures. By means of a kinetically controlled electroless deposition process, the nanopore inner walls were uniformly coated with thin films of gold, platinum, palladium, platinum-ruthenium, platinum-palladium, and palladium-coated nickel, leading to respective nanotubes embedded in the polymer foil. This has been evidenced by cross-sectional SEM and TEM investigations.
Embedded Pd nanotubes were tested for their performance as catalyst for a flow-through reactor. In UV-Vis absorption spectrometric measurements, they showed a very high efficiency towards the nitrophenol reduction to aminophenol, used for the fabrication of paracetamol (acetaminophen), the well-known analgetic and antipyretic [1]. The nanotubes show an advantage over comparable nano particle based systems: in contrast to the latter, they are more mechanically stable and do not agglomerate, leading to a better long-term stability of the catalyst.
When the ion beams tracks in the polymer foil are crossed and the resulting nanopores are coated with metal, the dissolution of the polymer foil leads to free standing porous nanotube networks. Due to the cross-linking, they are mechanically very stable, despite the very small diameter of the individual nanotubes. With their large internal surface area, they constitute highly efficient catalysts for the methanol oxidation in Direct Methanol Fuel Cells. This has been shown for Pt-Pd alloy and Pd-doped Ni networks by means of electrochemical half-cell methanol oxidation measurements [2, 3].

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / **23**

On the modelling of Joule-Thomson Effects: Analytical and Numerical Formulations

Authors: Cintia Goncalves Machado[1]; Paul Egberts[1]; Negar Khoshnevis Gargar[1]

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Expansion and compression of fluids by injection or production in the reservoir leads to cooling or heating effects due Joule-Thomson and adiabatic processes. This effect on the near-wellbore temperature becomes significant in some applications such as carbon dioxide storage in a depleted gas reservoir. Commercial reservoir simulators using a compositional approach can model these effects. However, setting up and running compositional simulations can be very cumbersome and computationally costly, making it difficult to incorporate these simulations in workflows for uncertainty quantification, history matching and optimization. In order to allow incorporation of carbon dioxide injection modelling in workflows and networks, while keeping the relevant physics, we have derived two simplified models that account for Joule Thomson effects. The first is an analytical model based on solving for temperature and pressure equations with variable rate assuming a cylindrically shaped homogenous reservoir. In this case temperature and pressure are decoupled. This model calculates first the temperature profile based on the energy balance, and then computes the bottom hole pressure by integrating the pressure gradient given by Darcy's law for the different viscosity regions in the reservoir. We found an excellent match of this analytical model with a commercial reservoir simulator. The second model, a numerical model, allows for more complex geological features and fluid properties modelling. We have extended an open-source fully implicit black-oil thermal reservoir simulator to account for Joule-Thomson effects. We have compared the two-models against an industry-standard compositional simulation.

Participation:

In-Person

References:

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MS06-A / 24

Rheology and Mobility Critical Exponent of Immiscible Two-Phase Flow in Porous Media with Dual-Wettability Grains

Author: Hursanay Fyhn[1]

Co-authors: Santanu Sinha [2]; Alex Hansen [1]

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A large class of porous media consists of consolidated grains. If there is a mixture of different grain types, capillary forces may be strongly affected under immiscible two-phase flow. We have studied the effect of a random mixture of two types of grains having different wetting properties on the transport properties of immiscible two-phase flow in porous media under steady-state flow conditions using a dynamic pore-network model.

Immiscible fluids A and B flow through pores between two types of grains denoted "$+$" and "$-$". Fluid A is fully non-wetting with respect to grain type "$+$" and is fully wetting with respect to grain type "$-$". Fluid B is fully wetting with respect to grain type "$+$" and is fully non-wetting with respect to grain type "$-$". We model the pore structure as the links in a square lattice. The nodes of the dual lattice is populated by the grains. The grains of type "$+$" are assigned with a certain probability and the rest of the grains are assigned type "$-$". There are no spatial correlations among the grains. If a link passes between two "$+$" type grains, the capillary force at fluid interfaces in the link will point in the direction of fluid B. If a link has type "$-$" grains as neighbors, the capillary force at fluid interfaces in the link will point towards fluid A. If the link lies between type "$+$" grains on one side and type "$-$" grains on the other side, we assume the capillary force to be zero between the two fluids.

For a window of grain occupation probability values, a percolating regime appears where there are active connected paths with zero capillary forces. Due to these paths, no minimum threshold pressure is necessary to start a flow in this regime. Furthermore, while varying the pressure drop across the porous medium from low to high in this regime, the relation between the volumetric flow rate in the steady state and the pressure drop goes from being linear to a power law with an exponent 2.5, then being linear again. The linearity in the initial low pressure drop regime is due to the active connected paths with zero capillary pressures, which remains the same with small increase in the pressure drop. The non-linearity at the intermediate regime is due to the opening of new paths with the increases in the pressure drop whereas the linearity in the high pressure regime is essentially due to the entire network being active.

We also measure the mobility of the system at the percolation threshold of the grain occupation probability, which exhibits a critical behavior reminiscent to the conductivity of a random resistor network. We measure the critical exponent related to this mobility and find it approximately equal to 5.7.

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References:

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Energy Transition Focused Abstracts:

25

Application of CO2 huff-n-puff Enhanced Recovery and Geological Storage Technology in Santang Lake Oilfield

Author: Yangyue Xiang[1]

[1] *China University of Geosciences*

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The Carbon capture,utilization and storage(CCUS)technology is an effective means of reducing carbon emissions and an important supporting technology for achieving China's carbon peaking and carbon neutrality goals. The Carbon dioxide(CO2)flooding,namely the application of CCUS for enhanced oil recovery(CCUS-EOR),is one of the main CO2 utilization methods in this regard. Here are many methods by which CO2 can be injected. One of the most common methods, especially in unconventional reservoirs, is CO2 huff-n-puff. CO2 huff-n-puff process holds great potential to increase oil recovery and has a chance to sequester CO2 to reduce environmental footprint.

As an important component of unconventional oil and gas, tight oil is typically characterized by low porosity (<10%) and low permeability (<0.1 mD). Even with the high oil production rate, the oil recovery factor remains low at an estimated average 7%, which is far lower than compared to the rates conventional reservoirs. There is still a large amount of oil remaining in place. It has aroused wide interest in the application of Enhanced Oil Recovery (EOR) techniques, especially CO2 and gas injection EOR. In this case, it is necessary to evaluate the CO2 Huff-n-Puff EOR method to maximize the oil recovery factor.

For such simulation studies, compositional simulation is widely used to deal with the relevant physics, such as fluid and reservoir properties. However, the substantial computational burden makes it challenging to conduct the field case model with multiple hydraulic fractures and comprehensive well controls. Some important underlying physics might be masked due to the over-simplification of the simulation models, like complex fracture geometries which are often created during the hydraulic fracturing process and various hydraulic fracture height in different layers. In order to overcome these issues, a state-of-the-art embedded discrete fracture model (EDFM) was developed. The EDFM method can conveniently model complex fractures.

In this study, the component model is used to simulate the process of CO2 huff-n-puff in combination with the actual reservoir and fluid properties of Santanghu tight oil reservoir. Using the field production data of a horizontal well in this area, the EDFM method is used to verify the reservoir model. After history matching, the main influencing factors of CO2 flooding and storage capacity are studied.

In this study, a component model was used to simulate the CO2 huff-n-puff process in combination with the actual reservoir and fluid properties of the Santang Lake tight oil reservoir. The reservoir model was validated using the EDFM method using field production data from a horizontal well in the area. After further history matching, the main influencing factors affecting the CCUS-EOR as well as geological storage are investigated.

Participation:

Online

References:

Kim, T.H., Cho, J., Lee, K.S., 2017. Evaluation of CO2 injection in shale gas reservoirs with multi-component transport and geomechanical effects. Applied Energy 190, 1195–1206. https://doi.org/10.1016/j.apenergy.2017.01.047

Xiang Yong,Hou Li,Du Meng,Jia Ninghong,Lu Weifeng. Research progress and development prospect of CCUS-EOR technologies in China. Petroleum Geology and Recovery Efficiency 1–17. https://doi.org/10.13673/j.cnki.cn37-1359/te.202112048

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Wang, L., Tian, Y., Yu, X., Wang, C., Yao, B., Wang, S., Winterfeld, P.H., Wang, X., Yang, Z., Wang, Y., Cui, J., Wu, Y.-S., 2017. Advances in improved/enhanced oil recovery technologies for tight and shale reservoirs. Fuel 210, 425–445. https://doi.org/10.1016/j.fuel.2017.08.095

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MS09 / **26**

Deep learning aided pore scale modelling

Authors: Mostaghimi Peyman[None]; Wang Ying da[None]; Tang Kunning[None]; Armstrong Ryan[None]

Corresponding Authors: ryan.armstrong@unsw.edu.au, peyman@unsw.edu.au, kunning.tang@unsw.edu.au, yingda.wang@unsw.e

Pore scale imaging and modelling have played an enormous role in advancing knowledge in complex transport phenomena within porous media. We discuss new challenges and directions in pore-scale research by integrating artificial intelligence. These include the recreation of porous media images at a super-resolution, multimineral segmentation and prediction of petrophysical properties with applications in underground reservoir simulation, ore characterisation and groundwater modelling.

Participation:

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Energy Transition Focused Abstracts:

MS09 / **27**

Pore-scale modeling of pore-clogging by aggregation of particles

Author: Laurez Maya[1]

Co-authors: Cyprien Soulaine [2]; Philippe Leroy [3]; Laurent ANDRE [3]

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The injection of cold water into the subsurface to recharge the aquifer during the exploitation of geothermal resources mobilizes fine particles (colloids) which can detach, precipitate, or even deposit irreversibly clogging the porous formation at the vicinity of the well. These processes very often lead to a reduction in the operating time of the wells and additional operating costs are required in order to separate and remobilize the aggregates thus formed. At the reservoir-scale, these processes are described using CFT (Colloidal Filtration Theory) and the Kozeny-Carman relationship. Such models, however, rely on heuristic parameters which have to be tune to fit with experimental datas, which limit their predictive capabilities.

In this work, we developed a numerical code for the transport of colloidal particles at the pore scale. The code relies on a four-way unresolved-resolved CFD-DEM (Computational Fluid Dynamics - Discrete Element Method) coupling that includes hydro-mechanical interactions (e.g. collision, drag, lift, gravity) and electro-chemical interactions (e.g. Van der Waals attraction and electrostatic double layer repulsion commonly known as DLVO (Derjaguin-Landau-Verwey-Overbeek) forces) between the particles, the fluid and the porous formation. The code, implemented within the open-source platform OpenFOAM, has been verified on cases for which reference solutions exist. We use the numerical model to investigate the deposition/remobilisation kinetics and the permeability/porosity relationship at the pore-scale under various flow, particle size and concentration, pH and salinity conditions. These new insights into the transport and deposition of colloidal particles in porous media will guide the development of reservoir-scale models rooted in the elementary physical principles.

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In-Person

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MS11 / 28

Insights into pore-scale hydrate morphologies during formation and dissociation in microfluidic for CH4 hydrate exploitation

Author: Qian Ouyang[1]

Co-authors: Jyoti Shanker Pandey [1]; Nicolas von Solms [1]

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Natural gas (main methane CH4) hydrates are such a prospective energy resource that feeds the global energy demand. Depressurization has been proved the most economical method for CH4 hydrate exploitation. However, micro characteristics of hydrate distribution and fluid migration in porous media are still lacking for efficient CH4 hydrate exploitation. In this work, morphologies of CH4 hydrate formation in synthesis and dissociation in exploitation were investigated in microfluidic chip resembling sandstone. During hydrate synthesis, morphological results showed CH4 hydrate nucleated at gas-water interfaces, and hydrate nucleation is much more apparent at dynamic fluid flow. The hydrate nuclei then grew towards gas phase, changing from coarse patterns to smooth ones by consuming CH4 gas. During hydrate exploitation, gas bubbles emerged in hydrate phase after dissociation pressures reduced to or below CH4 hydrate equilibrium pressure. Hydrate reformation was observed during depressurization because of localized pressure variation as a result of fluid migration. Pressure differences between inlet and outlet existed and after its disappearance, scattered gas bubbles merged into gas flow, depending on constant-rate of depressurization and mass transfer barriers in different pores. Higher initial water saturation triggered more coarse hydrates during formation, which turned into crystal patterns acting as barriers for mass transfer. Pore surface wettability and pore size exerted a significant effect on fluid appearance and distribution during hydrate dissociation. These micromorphology findings are beneficial to understand the mechanisms of hydrate transitions in confined porous media and thus provide insights for efficient CH4 hydrate exploitation through controlled depressurization.

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Poster / 29

An innovative method for the utilization of quarry sand

Authors: Dorina Strieth[1]; Niklas Erdmann[1]; Susanne Schäfer[2]; Eva Hagen[1]; Ulrich Bröckel[3]

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50 % waste (quarry sand) is generated during the production of ashlar. In this study, this waste material is used to produce biosandstone as new and sustainable construction material. The quarry sand

used in this study is delivered by the local natural stone plant (Picard) in Krickenbach (Germany). Viewed globally, there is a high need to investigate new construction material as alternatives to concrete, because with a share of about 8.6 % of anthropogenic CO2 emissions, concrete is a major contributor to global warming. Additional, not every sand like for example sand from the desert can be used for the production of concrete because the supporting grain is missing. Microbiologically induced calcium carbonate precipitation (MICP) offers the potential of a more sustainable alternative in construction. Additional, pretrials showed that a consolidation of sand from different deserts is possible allowing desert sand to be used as an alternative building material. During MICP calcium carbonate is formed by microbiological activity and can serve as a binder between mineral particles. This calcium carbonate can be an alternative binder to conventional cement mortar used for concrete. The most commonly used mechanism for MICP is ureolysis. In this process, a cell suspension and a calcination solution (urea + calcium ions) are applied alternately in a cyclic process, whereby calcium carbonate crystals are formed by the metabolism of the cells, which bind the aggregate (e.g.: sand) together.
In this study, Sporosarcina pasteurii is used as ureolytic microorganism to consolidate the quarry sand from the local natural stone plant in Krickenbach. In a first step, the quarry sand was consolidated by MICP to check if this is possible at all. Since this was successful, a deeper understanding of the influence of particle size on consolidation was investigated. Therefore, the quarry sand was classified into four different fractions of particle sizes and consolidated using MICP. In addition, the consolidated samples were scanned by micro computed tomography. Contact points and pore space depending on various parameters during the treatment of MICP were investigated. However, this study shows what influence the grain size has on the strength of the biosandstone. Furthermore, it will be shown what influence the pore volume has on the strength of the samples and whether the strength can be optimized by an optimal composition of the different fractions of particle sizes. Finally, a demonastrator will be presented produced from quarry sand using the interlocking principle. The interlocking principle is an adaptable modular structure based on the building block principle, which is functional without mortar.

This project is financially supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) –Project-ID 172116086 –SFB 926, the “Landespotentialbereich NanoKat”and “Lehre Plus”.

Participation:

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Energy Transition Focused Abstracts:

MS01 / 30

The Impact of Capillary Heterogeneity on CO2 Plume Migration at the Endurance CCS Target Site in the UK –A Core To Field Scale Study

Author: Nele Wenck[1]

Co-authors: Samuel Jackson [2]; Ann Muggeridge [1]; Sam Krevor

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[2] *CSIRO*

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The characterisation of multiphase flow properties is key to predict large-scale fluid behaviour in the subsurface, such as the migration of a carbon dioxide (CO2) plume at a Carbon Capture and Storage (CCS) site. Many CCS sites have displayed unexpected fluid flow behaviour, where the CO2, once injected, migrated away from injection wells at significantly higher rates and in different orientations to what had been predicted with reservoir simulations. Recent studies have demonstrated that conventional reservoir models are not incorporating the impact of small-scale heterogeneities in multiphase flow properties, such as capillary heterogeneity. In this work, we combine experimental and numerical methods to model the impact of capillary heterogeneity on CO2 plume migration at the proposed Endurance storage site. The site supports the Northern Endurance Partnership (NEP) serving the Zero Carbon Humber and Net Zero Teesside projects in the UK. We build small-domain, fine-scale models, populated with well and experimental data from the Endurance site. These models are used to infer the impact of heterogeneity on CO2 flow in 3D with the full physics represented. Our results show that capillary heterogeneity can lead to a 3-fold increase in the relative CO2 migration speed, underscoring the importance of characterising and incorporating it within reservoir models. Using the results, we then build a full field-scale 3D model of the Endurance site. We apply a novel upscaling scheme, originating in the work of Jackson & Krevor (2020), to model the impact of heterogeneity, buoyancy and structure on CO2 migration. Our results emphasize the prevalent impact of small-scale capillary heterogeneities on CO2 plume migration.

Participation:

In-Person

References:

Jackson, S. J., & Krevor, S. (2020). Small-scale capillary heterogeneity linked to rapid plume migration during CO2 storage. Geophysical Research Letters, 47, e2020GL088616. https://doi.org/10.1029/2020GL088616

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MS03 / **32**

Linkage between extended poroelasticity and micromechanics

Author: Filip Adamus[1]

Co-authors: David Healy [2]; Phil Meredith [3]; Tom Mitchell [3]

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We attempt to formalise the relationship between the poroelasticity theory and the effective medium theory of micromechanics. Assumptions of these approaches vary, but both can be directly linked by considering the undrained response of a material. To analyse the linkage between poroelasticity and micromechanics, we do not limit ourselves to the original theory of Biot. Instead, we propose a concise extension of anisotropic poroelasticity, where pore fluid pressure may vary within the representative volume element. As a consequence, the inhomogeneities are not necessarily interconnected—they may form separated pore sets that are described by distinct poroelastic parameters and pore pressure. Further, we attempt to incorporate the effective methods inside Biot-like theory and investigate the poroelastic response of various microstructures. We show the cases where such implementation is valid and the others that appear to be questionable.

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MS21 / 33

Immersion of porous aggregates: application to concrete recycled aggregates

Authors: Emmanuel Keita[1]; Florian Thérénéé[None]; Jennifer Naël-Redolfi[2]; Pascal Boustingorry[2]; Nicolas Roussel[3]

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Due to the limited resources of alluvial aggregates, the use of recycled aggregates has become a growing practice in the construction industry today. These recycled aggregates come from the recycling of building or road demolition waste. They differ from natural aggregates in their composition and structure. The high porosity of this hardened cement paste implies a high-water absorption, which can reduce the workability and modify the properties of hardened concrete.
This presentation investigates the water transfers between porous aggregates and fresh cement paste. First, sintered glass beads are used as a model porous media; similarly, the cement paste is replaced by water to identify the dominant physical phenomena better.
We thus show the influence of the geometry and microstructure of the porous medium on the imbibition kinetics by immersion in water. Therefore, the commonly used Washburn model must be adapted to describe the imbibition kinetics. Geometry-specific imbibition models are then developed.
In the second step, we characterize the water transfer between the fresh cement paste and the porous aggregates. By Nuclear Magnetic Resonance spectrometry (NMR), we show that the absorption of

aggregates in fresh cement paste is lower than in pure water. This decrease in absorption is a consequence of the contraction of the fresh cement paste during imbibition. Furthermore, the absorption kinetics is also slowed down compared to the measurements in water.

Participation:

In-Person

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MS05 / **34**

Impact of the internal heterogeneity of biofilms on hydrodynamics and reactions in 3D porous media

Authors: Ishaan Markale[1]; Maxence Carrel[2]; Dorothee Luise Kurz[1]; Veronica Morales[3]; Markus Holzner[4]; Joaquin Jimenez-Martinez[1]

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Bacterial biofilms can form in porous systems that are of interest in industrial but also in environmental applications, being hotspots of biogeochemical reactions. The presence of biofilms within porous media modifies not only the topology but also the hydrodynamics and consequently the transport of solutes and the effective kinetics of reactions. The highly heterogeneous flow fields found in porous media during biofilm growth translate into a spatially heterogeneous biofilm location and internal heterogeneity. Using highly resolved three-dimensional X-ray computed microtomography images of bacterial biofilms in a porous medium, multiple equivalents stochastically generated internal permeability fields for the biofilm are generated. These permeability fields embedded within the porous medium are used to compute pore-scale fluid flow and solute transport numerically. We observe that the biofilm with an internal heterogeneous permeability mainly impacts intermediate velocities when compared with a homogeneous case. The equivalent internal permeability fields of the biofilm do not impact fluid-fluid mixing. However, they significantly control a fast fluid-fluid reaction. For biologically driven reactions such as nutrient or contaminant uptake by the biofilm, its internal permeability field enhances the process, especially at early times. This study highlights the importance of considering the internal heterogeneity of biofilms to better predict reactivity in industrial and environmental bioclogged porous systems.

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Energy Transition Focused Abstracts:

MS06-B / 36

Exploring the Influence of Interfacial Processes on the Transport and Retention of PFAS in AFFF-Contaminated Soils

Author: Linda Abriola[1]

Co-authors: Uriel Garza Rubalcava [1]; Craig Klevan [1]; Kurt D. Pennell [1]

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Per- and Polyfluoroalkyl Substance (PFAS)-containing Aqueous Film Forming Foams (AFFFs), employed in firefighting, have been recognized as a major source of PFAS contamination across the globe. In addition to the release of PFAS-containing solutions, firefighting training and emergency response activities have also typically involved the intentional or accidental co-release of hydrocarbon fuels and chlorinated solvents (nonaqueous phase liquids (NAPLs)), creating complex contaminant mixtures. Due to their amphiphilic properties, PFAS accumulate at interfaces, and thus, the presence of air-water, soil-water, and NAPL-water interfaces within these release areas can influence both the transport and distribution of PFAS in the subsurface. This presentation provides an overview of recent collaborative research related to the development, validation, and application of mathematical models that describe the transport and retention of PFAS mixtures in complex AFFF-contaminated source areas. Modeled processes include interfacial accumulation, interfacial tension reduction and associated moisture redistribution, nonlinear sorption to the solid phase, and competitive sorption/interfacial accumulation effects. Data from interfacial tension and batch sorption measurements are used in conjunction with moisture retention curves and experimental observations from multi-phase column experiments to assess model performance. Here, a Langmuir-Szyszkowski equation is employed to model surface excess of individual PFAS, and fitted single solute parameters are employed, in an extended Langmuir isotherm framework, to predict competitive interfacial accumulation for PFAS mixtures. Experimental measurements and model simulations of PFAS transport in two-phase (NAPL-aqueous and air-aqueous) fluid systems demonstrate the influence of interfacial tension reduction and competitive adsorption phenomena on anomalous transport behavior in clean sands. The validated model provides a comprehensive tool to explore the influence of interfaces on PFAS mixture fate and transport in subsurface environments. Example applications to field-scale AFFF release scenarios illustrate the potential influence of release history, soil texture, and PFAS characteristics on the spatial distribution of contaminants within the unsaturated zone and on contaminant migration to the water table.

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MS08 / **37**

A Geo-structurally Based Correction Factor for Apparent Dissolution Rates in Fractured Media

Author: Jeffrey Hyman[1]

Co-authors: Alexis Sitchler [2]; Bill Carey [1]; Satish Karra ; Hari Viswanathan [1]; Matthew Sweeney [3]; Elizabeth Andrews [4]

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Field measurements of apparent geochemical weathering reaction rates in subsurface fractured porous media are known to deviate from laboratory measurements by multiple orders of magnitude. To date, there is no geologically based explanation for this discrepancy that can be used to predict reaction rates in field systems. Proposed correction factors are typically based on ad hoc characterizations related to geochemical kinetic models. Through a series of high-fidelity reactive transport simulations of mineral dissolution within explicit 3D discrete fracture networks, we are able to link the geo-stuctural attributes with reactive transport observations. We develop a correction factor to linear transition state theory for the prediction of the apparent dissolution rate based on measurable geological properties. The modified rate law shows excellent agreement with numerical simulations, indicating that geological structure could be a primary reason for the discrepancy between laboratory and field observations of apparent dissolution rates in fractured media.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / **39**

Numerical simulation of hydraulic stimulation on geothermal reservoirs: injection optimization to manage induced seismicity and thermal decline

Authors: Sandro Andrés Martínez[1]; David Santillan Sanchez[2]; Juan Carlos Mosquera Feijoo[1]; Luis Cueto-Felgueroso[2]

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Geothermal energy is a renewable resource that may help to provide a green energy supply, although the low rock permeability at the required depth prevents an energy-efficient use of this resource. Enhanced Geothermal Systems (EGS) allow to increase permeability by means of the hydraulic stimulation of the fractures of underground formations. However, it implies risks as, for instance, induced seismicity or an early thermal exhaustion of the reservoir.

We perform numerical simulations to delve into the thermo-hydro-mechanical and frictional phenomena that control that risks in EGS projects. Our computational model solves the fully coupled equations of thermo-poro-elasticity, together with rate-and-state friction at faults. The methodology allows us to simulate both fluid-injection induced earthquakes and long-term behavior of geothermal reservoirs.

In the short them, we explore the optimization of the injection protocols to avoid or delay fault reactivation. Our results arise that the injection protocols with an early increase of flow rate could delay fault reactivation depending on the frictional properties of the contact. In the long term, we observe that the permeability stimulation can induce an early thermal decline of the reservoir. This may affect to energy production over years, depending on the increase of permeability achieved with hydraulic stimulation.

The methodology proposed in this work may help to improve the competitiveness of geothermal energy, as it can be a useful tool to manage the seismic risk and the long-term operation of geothermal reservoirs.

Acknowledgements

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Participation:

In-Person

References:

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Poster / 40

Microscopic production characteristics and influencing factors of micro-nano pores in shale oil enhanced oil recovery by air injection

Author: Meng Du[None]

Co-authors: zhengming yang [1]; weifeng lv ; Lanlan Yao ; Xinliang Chen ; yilin chang ; Liang Ma

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Abstract: In order to explore how to improve the development effect of air flooding in shale oil, an online physical simulation method for shale oil air injection enhanced oil recovery was established by high-temperature and high-pressure CT scanning and nuclear magnetic resonance (NMR) technology, the development effect of air flooding of shale oil under different depletion pressures and the micro-production characteristics of different pore throats were analyzed, and the oil recovery mechanism of shale oil air flooding was given. On the basis, the effects of air oxygen content, permeability, capillary number, and gas injection pressure on the shale air flooding effect and pore crude oil production were analyzed. Subsequently, the shale digital core pore-fracture network model was reconstructed by high-resolution CT combined with advanced algorithms of AVIZO visualization software, and the influence of fracture development degree on enhanced oil recovery was analyzed by combined with magnetic resonance imaging (MRI). The results show that the development effect of shale oil could be greatly improved by injecting air after the shale reservoir was depleted, but the oil displacement efficiency and the production degree of different levels of pore throats under different injection timing were different. At the initial state, the crude oil in the shale core was mainly distributed in nanopores, sub-micropores, and micropores, where the oil content exceeded at least 75% in these pores. The oil discharge rate of macropores was fast at first and then slows down, but the oil discharge rate of nanopores increased almost linearly during air flooding. The higher the air oxygen content, the stronger the low temperature oxidation, the more obvious the thermal effect and the viscosity reduction effect, the higher the production degree of pores at different levels, and the recovery factor gradually increases. The higher the permeability, the better the pore throat connectivity, the stronger the fluid flow capacity, and the higher the recovery degree of shale oil. With the injection pressure increases, the lower limit of the minimum pore throat production increases, but it is easy to produce gas channeling, which leads to the breakthrough in advance, and the recovery increases first and then decreases. Notable, fractures can effectively increase the contact area between gas and crude oil, promote the mass and heat transfer between matrix fractures, and increase the air sweep coefficient and matrix oil drainage area by supplying oil to fractures through the matrix; the utilization of submicron pores and micron pores increased to 34.3% and 42.7%, respectively, which means that the proper fracturing before air injection can help to improve the oil displacement effect of air injection.

Key words: NMR; shale oil; heat and mass transfer; air flooding; CT scanning; EOR; microscopic production; factor

Participation:

In-Person

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MS09 / 41

Geometrical analysis of the pore space through the A* algorithm: application to 3D micro-CT images

Author: Filippo Panini[1]

Co-authors: Eloisa Salina Borello [1]; Dario Viberti [1]

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The definition of an optimal reservoir management strategy is fundamental for the primary production of oil and gas, Enhanced Oil Recovery, Underground Gas Storage, Underground Hydrogen Storage, CO2 storage, and geothermal systems. Due to the complexity of geological formations, the uncertainty associated to the fluid-rock interaction parameters must be estimated and possibly mitigated by the acquisition of further information at all stages of reservoir life. The characterization and analysis of fluid flow phenomena at the pore scale can contribute to minimizing such uncertainties. Thanks to micro-CT images, a realistic representation of the reservoir rock is obtained, and it can be used as input for further analyses of pore space characteristics. In this work, the A* search algorithm (Hart et al., 1968) is used to compute the shortest connected paths across micro-CT images of rocks in the three main flow directions. This information is employed to calculate tortuosity, effective porosity, constriction factor, pore size distribution, permeability and anisotropy ratio of the rock. This process was introduced by Salina Borello et al. (2022) but was not applied to real 3D images of rocks obtained by micro-CT techniques. In this work, a sandstone and two carbonate rocks are analyzed. Fluid flow is intrinsically influenced by all the features of the pore space (i.e. tortuosity, effective porosity, constriction and pore radius) and the porous medium is usually characterized by a single parameter, the permeability, which takes into account all these properties. In fluid flow simulation, permeability can be calculated directly by inverting the Darcy's law. In the geometrical analysis instead, all pore space characteristics are evaluated individually and combined through the Kozeny-Carman equation. The geometrical tortuosity is calculated as the average length of the shortest (or geometrical) paths divided by the edge length of the sample. The effective porosity is

computed as the portion of pore space crossed by the geometrical paths. The constriction factor expresses the variation of the pore cross-section orthogonal to the path. The pore size is estimated as the distance between the pore walls locally orthogonal to the path. In order to calculate the permeability, the Kozeny-Carman equation is used by including the geometrical tortuosity, effective porosity, and a representative pore radius in the equation. Finally, the anisotropy ratio is calculated using permeability values in the three main directions. Results are compared with those obtained by single-phase CFD simulation directly in the pore space using OpenFOAM, with the exception of pore size distribution and constriction factor. Geometrical analysis and CFD simulations are run at the pore-scale directly on binary images of rocks. The values of tortuosity, effective porosity, permeability, and anisotropy ratio calculated with the geometrical analysis and CFD simulation are in good agreement in all the cases. The outcome of this investigation evidences that the geometrical analysis used in this research can provide a reliable characterization of rocks.

Participation:

In-Person

References:

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MS15 / **42**

Machine Learning for the Characterization of Fibrous Gas Diffusion Layers for Polymer Electrolyte Fuel Cells

Authors: Dieter Froning[1]; Eugen Hoppe[2]; Ralf Peters[2]

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The permeability of gas diffusion layers (GDLs) depends on their micro-structure, and is relevant for transport simulations at higher scales, e.g., fuel cells and stacks. Given the micro-structure, the permeability can be obtained from transport simulations [1], which typically requires large computing
resources. Such GDLs are used in polymer electrolyte fuel cells (PEFCs), as well as in some electrolysers.
Drawing on previous published simulations [1] of gas flow through fibrous GDLs, a convolutional neural network (CNN) was trained [2, 3]. The underlying data were based on a stochastic geometry model that also featured different binder models and compression levels. A small number of microstructures –541 –was sufficient for not only achieving good accuracy in the predicted permeability but
also for reproducing the binder type as a hidden feature that was not explicitly trained.

The training data for the CNN are micro-structures generated by means of a stochastic geometry model [1]. The fibers with a diameter of 7.5 µm were created layer-wise. The fiber orientation is stochastically-equivalent to the real structure of Toray 090 material, which was validated using X-ray
synchrotron imaging [1]. An additional binder was added using four kinds of binder sub-models. The
resulting micro-structures were provided in both uncompressed and compressed forms. The output feature –label data for the CNN –was the through-plane permeability of the GDL, calculated by means
of Lattice–Boltzmann simulations of single-phase flow through the micro-structure. Because the LB simulations required large computational resources, it was intended to take a limited number of these to
train a CNN that can predict permeability with sufficient accuracy. This was achieved using historical
data from previous investigations [1]. Validated with five-fold cross validation, the CNN was able to predict the permeability with an accuracy greater than 5% for uncompressed micro-structures, as well
as relevant compression levels [3]. Although the binder type was not provided for training the CNN, this hidden feature was reproduced by the predictions using the trained CNN.
The calculation of the permeability of the micro-structures required high-performance computers (HPCs); the training of the CNN also requires large computational resources, preferably GPU-based ones. With a trained CNN, the prediction of permeability can be run on a standard computer.
Transport simulations were run on the hardware of the Jülich Supercomputing Centre, grant: CJIEK30.
The neural network was trained on GPU nodes of the CLAIX system at RWTH Aachen University, using grants jara0070 and p0020317.
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Hyperbolic Systems for Strongly Coupled Multi-Phase Flow and Transport in the Sub-Surface

Authors: Patrick Jenny[None]; Rasim Hasanzade[1]; Hamdi Tchelepi[None]

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Multiphase flow and transport in porous media typically is simulated by solving an elliptic or parabolic flow equation together with hyperbolic transport equations. In case of tight coupling, either a fully implicit solution algorithm is required, or very small time steps have to be employed, if a sequential algorithm is used. Here, a new solution approach is presented, which relies on a coupled hyperbolic system of conservation laws. Latter can efficiently be solved with an explicit finite volume method, which is advantageous in many ways, since all operations are local. The hyperbolic system is based on the isothermal Euler equations with momentum source terms accounting for resistance due to the porous medium as well as for buoyancy. Further, to account for saturation transport, the system was augmented by an additional hyperbolic equation. If the parameters are chosen such that the Mach number is much less than one and inertia remains small compared to the momentum source term, the obtained results converge to the same solutions as obtained with a classical reservoir simulator. To compute the numerical fluxes, a characteristic based approximative Riemann solver was developed and 2nd order accuracy in space and time is achieved by piecewise linear reconstruction. As demonstrated with numerical experiments, the devised method is very promising and well suited for massive parallel computations.

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MS22 / 45

MOF sensors for contaminant capture and detection: cooperative computational-experimental screening approach

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The remarkable mastery over chemical synthesis in the modern world has drastically enriched humanity. At the same time, our activity often results in significant emissions of undesirable contaminants, including toxic gases (NOx, SOx, CO), volatile organic compounds (BTEX, esters, aldehydes,

⋯) alongside other volatile compounds posing threats to both human health and sensitive machinery. Therefore, the detection and abatement of airborne contaminants at low levels (ppb to ppm) is an ongoing challenge for maintaining a clean and safe environment, particularly in regulated spaces, such as clean rooms, satellites, and indoor living spaces.

In this context, framework materials like MOFs and COFs appear as promising materials due their tailorable chemical and physical properties and highly porous structures, acting as sorption media for direct air capture of contaminants,[1] or as components in electronic devices designed for monitoring their concentration.[2] Nevertheless, given the large number of synthesizable frameworks [3] the choice of a material to target a specific contaminant is more often than not a question of serendipity.[4]

To overcome this problem, a generalized approach is herein given for screening MOFs for specific contaminant molecules. This method combines high-throughput molecular simulations to highlight key promising materials, followed by advanced adsorption experiments at very low contaminant concentrations and sensing. We further detail several classes of MOF materials which were identified through this approach that are applicable to the capture and detection of common contaminants in the space industry (i) siloxanes, (ii) aromatics and (iii) esters.

Participation:

In-Person

References:

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MS03 / **46**

Multiscale poromechanical model for naturally fractured coal seam reservoir considering non-linear fracture deformation and adsorption effects

Authors: Quoc Dat Ha[1]; Tien Dung Le[1]; Irina Panfilov[1]; Christian Moyne[1]; A. Marcio Murad[2]

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In this work, a three-scale poromechanical model for naturally fractured coalbed methane reservoir is developed. The coal seam reservoir is composed of a coal matrix mainly containing nanopores

saturated by adsorbed gases and natural fracture network (called cleats). Beyond the empirical Langmuir law, the adsorption isotherm of the fluid mixture (CH4 and CO2) is rigorously constructed by using the Density Functional Theory (DFT) applied to a Lennard-Jones fluid [1, 2, 3], allowing to compute the fluid distribution in the pores and the adsorption-induced force (solvation force) exerting on the solid phase by the adsorbed fluid. It is highlighted that the solvation force magnitude is much higher than the bulk pressure leading to an important impact on the mechanical properties at higher scale. A first homogenization procedure of the nanopore scale model is performed to derive the mechanical response of the continuum matrix, characterized by a modified Biot-Willis parameter depending on the solvation force magnitude. Such system of governing equations in the matrix is coupled with the fluid pressure in the discrete cleat system with dependency of aperture with the normal stress dictated by the hyperbolic Barton-Bandis model [4]. The problem is strongly non-linear and coupled with the hydrodynamics due to the rapid increase of the joint stiffness and the dependence of the fluid pressure. Moreover, the cleat stiffness is directly related to the cleat closure, which controls the permeability of the reservoir. A second homogenized procedure is pursued and capable of providing the constitutive response of the homogenized poromechanical parameters on gas pressure at the reservoir scale. In this context, increase in the normal BB-stiffness of the cleats tends to reduce the jumps of characteristic functions at the matrix/cleat interfaces which are propagated to the macroscale in terms of perturbations in the macroscopic poromechanical parameters. In addition to the overall three-scale decomposition of the total macroscopic stress, we constructed a new constitutive law for the Lagrangian cleat porosity. The dependence of the two- and three-scale homogenized poromechanical coefficients on the gas pressure is reconstructed numerically quantifying precisely the influence of the solvation force and the non-linear elastic behavior of the natural fractures.

Finally, the poromechanics is coupled with the multiscale hydrodynamic model in order to simulate the enhanced coalbed methane reservoir by CO2 injection. The interplay between the solvation force due to the adsorption effect and the non-linear elastic response of the fractures is numerically analyzed during the CH4 production and the CO2 injection procedure, underlying the increase in fracture stiffness at the injection well due to the matrix swelling stemming from the preferential CO2 adsorption in coal. Moreover, the fracture permeability tends to decrease in the vicinity of the injection well due to the same effect.

Participation:

In-Person

References:

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Poster / 47

A hybrid MPM-CFD model for simulating multiphase flow in deformable porous media.

Author: Quoc Anh Tran[1]

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Presented here is a model of soil-fluid-structure interaction that integrates soil mechanics (saturated sediments), fluid mechanics (seawater or air), and solid mechanics (structures). As a result of this formulation, the Material Point Method, which simulates large deformations of the porous media and the structure, is combined with the Implicit Continuous-fluid Eulerian, which simulates complex fluid flows. Our model is validated and we simulate the entire submarine landslide process resulting from earthquakes. Using this model, we are able to estimate the impact of submarine landslides on offshore structures by taking into account the complex interactions between saturated sediment, seawater, and structures.

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Label-Free AI-Based Surrogate Modelling for Highly Compressible Subsurface Flow

Author: Victor Molokwu[1]

Co-author: Mahmoud Jamiolahmady [2]

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This paper presents an improved approach in developing artificial intelligence (AI)-based surrogate reservoir models (SRM) for highly compressible gas flow in porous media. The nonlinear dynamics exhibited by highly compressible gas flow are captured by the AI-based surrogate using both physics-based and non-physics-based regularization parameters and without the need for a labelled training dataset. A convolutional-based encoder-decoder neural network (CEDNN) is used as the core function the developed SRM. The CEDNN is coupled with other modular networks which include a pretrained polynomial layer and a fully connected deep neural network (FCDNN) with residual connections. The pretrained polynomial layer discovers the pressure-dependent fluid properties, and

the FCDNN with residual connections allows for adaptive timestep learning. The coupled network is trained in a weakly-supervised manner using both physics and non-physics-based regularization terms. The physics-based regularization terms are obtained from a discretized partial differential equation of the subsurface flow domain, as well as the initial and boundary conditions. The non-physics-based regularization term, which acts as smoother, is computed as the Euclidean norm of the network's trainable parameters and is implemented via a decoupled-weight decay first-order optimizer. The coupled network uses discriminative layer training which provides independent tuning for each of the network modules.
The AI-based SRM has been tested on a dry gas fluid, with a varying permeability field generated for 54 (training and validation) and 6 (testing) realizations. The considered flow domain has a single well with no-flow outer boundary and operating at different inner boundary. The model is run for 540 days at a 10-day timestep interval. The CEDNN predictions after the training are in good agreement when compared with results obtained from a numerical simulator. The time expense is during the training of SRM which takes about 50 mins. However, the full space-time test predictions are obtained in 2-3 seconds as compared to about 192 seconds (64 times) by the numerical reservoir simulator. The timeliness of the developed AI-based SRM during predictions proves to be an appropriate tool for sensitivity and uncertainty analysis.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS10 / **49**

Investigating the Use of Electrical Capacitance Tomography to Image Rapid Transient Moisture Flow Through Cracks in Concrete

Author: Laura Dalton[1]

Co-authors: Mikko Räsänen [2]; Antti Voss [2]; Aku Seppänen [2]; Mohammad Pour-Ghaz [3]

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[3] *North Carolina State University*

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In this study, we investigate the feasibility of Electrical Capacitance Tomography (ECT) to image rapid three-dimensional (3D) moisture transport in damaged portland cement mortar and concrete. ECT is a tomography method that uses inter-electrode capacitance measurements to reconstruct the internal 3D distribution of the electrical permittivity which carries contrast with respect to moisture content. In the experimental study, ECT measurements were performed with a reservoir placed directly on the crack in each specimen to promote rapid moisture transport to test the high temporal resolution capabilities. An electrode array connected to an electrical tomography device was used to

conduct moisture transport measurements in cracked specimens at a temporal resolution as high as 0.7 seconds. The results of this study illustrate that ECT can be used to detect rapid moisture transport through various crack patterns and capture the flow path of water around coarse aggregates as shown in Figure 1.

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In-Person

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Energy Transition Focused Abstracts:

MS03 / **50**

A generalised phase-field model for fluid-driven dynamic fracture propagation in porous media

Authors: Kou Du[1]; Alex Routh[None]

[1] *University of Cambridge*

Corresponding Authors: afr10@cam.ac.uk, kd515@cam.ac.uk

Hydro-mechanical coupling in deforming porous media has been the subject of studies in mechanical, energy, geology and environmental engineering. In our work, following Griffith's theory [1] and Francfort and Marigo's [2] variational approach to fracture, we develop a generalised phase-field-based formulation for predicting the fluid-driven fracture propagation in porous media across different time scales. The advantage of the phase-field method is that the complex fracture behaviour, such as initiation, propagation, branching and merging, is the natural outcome of simulations without prior knowledge of propagation path. A macroscopic framework is proposed for phase-field modelling of dynamic fracture to couple the physics of flow with the mechanics of fracture, including the deformation behaviour of solid skeleton, the crack propagation and fluid flow within pores and cracks. The effect of fluid properties such as viscosity and permeability is also discussed. The numerical algorithm is implemented in ABAQUS by user-defined subroutines. We compare numerical results against several analytical and experimental solutions and also demonstrate the approach' s ability to predict complex fluid-driven fracture systems.
[1] Griffith Alan Arnold & Taylor Geoffrey Ingram. The phenomena of rupture and flow in solids. Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character 221, 163–198 (1921).
[2] Francfort, G. A. & Marigo, J.-J. Revisiting brittle fracture as an energy minimization problem. Journal of the Mechanics and Physics of Solids 46, 1319–1342 (1998).

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS09 / **51**

Gyroid structures with topology-optimised mechanical properties designed by simulations

Authors: Leonie Wallat[None]; Michael Selzer[None]; Frank Poehler[None]; Britta Nestler[None]

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Triple periodic minimal surfaces can be approximated to three-dimensional cell structures, which are found in many forms in nature, such as on butterfly wings or on the skeletal plate of a sea urchin. The structures are representable by a mathematical periodic function. For sheet-based structures, the result is two disjoint, intertwined channels with a uniformly curved surface. The three most common sheet-based structures are D-gyroids, Schwartz diamonds, and Schwartz primitive structures.
The three-dimensional regular periodic structure makes them attractive for various research areas, such as in the medical field for tissue engineering or as a possible heat exchanger, due to their high surface to volume ratio, bionic and mechanical properties.
In this work, the sheet-based gyroid structures with different porosity-levels are topology optimized with respect to their mechanical stability at constant volume using the inhouse micro structure simulation framework “Pace3D”. The optimized structures and the original structures are simulated and compared with respect to their mechanics in the linear-elastic range, and other properties such as the surface-to-volume ratio are also investigated.
Simulations of mechanical load in the linear elastic regime are carried out on both the optimized as well as the original structures and the mechanical properties are compared. Furthermore, micro structure characteristics such as the surface-to-volume ratios are evaluated.

Participation:

In-Person

References:

Wallat L, Altschuh P, Reder M, Nestler B, Poehler F. Computational Design and Characterisation of Gyroid Structures with Different Gradient Functions for Porosity Adjustment. Materials (Basel). 2022 May 23;15(10):3730. doi: 10.3390/ma15103730. PMID: 35629755; PMCID: PMC9144873.

Leonie Wallat, Michael Selzer, Uwe Wasmuth, Frank Poehler, Britta Nestler. Energy absorption capability of graded and non-graded sheet-based gyroid structures fabricated by microcast processing. Journal of Materials Research and Technology,
Volume 21. 2022. Pages 1798-1810. ISSN 2238-7854. https://doi.org/10.1016/j.jmrt.2022.09.093.

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Energy Transition Focused Abstracts:

53

Young-Laplace equation in shale and nanopores

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Corresponding Authors: asakhaee@central.uh.edu, malipour@central.uh.edu

Since the economical production of oil and gas from shale formation and their potential to act as sealing for hydrogen storage and carbon dioxide sequestration, it has been the focus of considerable research. However, there are uncertainties in the applicability of existing methods for characterizing rock and fluid interactions because the pore size is on the order of a few nanometers, and pore proximity affects the physical properties of the fluid inside. The Young-Laplace relation is a relevant example for interpreting pore-throat size from capillary pressure measurements. This study presents a correction to the Young-Laplace equation to extend its application to shale formations and nanopores. The relative error of applying the conventional Y-L equation to calculate the pore-throat radius is also quantified. This study shows that 10 nm is a threshold size, which corresponds to the capillary pressure of 80.18 MPa in the mercury injection, for the pore throat below which it is necessary to apply a correction. . Pore-throat radius and distribution of shale formations in the US were calculated using the corrected Y-L. The relative error of conventional Y-L in 10 nm pores is 5% and increases to 20% in 2 nm pores. The presented correction has applications in estimating the pore-throat size distribution, entry pressure, and permeability of the shale formation from capillary pressure.

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Energy Transition Focused Abstracts:

54

A Microfluidic platform to study microbial activity in permafrost samples

Authors: Niloofar Fasaeiyan[None]; Pooneh Maghoul[None]; Lukas Arenson[None]; Richard Boudreault[None]

Corresponding Authors: richard@techaero.ca, pooneh.maghoul@polymtl.ca, larenson@bgcengineering.ca, niloofar.fasaeiyan@polymtl.ca

Microbial activity is considered a vital element in the biology of permafrost soils due to its critical role in regulating most soils functions, especially the amount of carbon (greenhouse gases) released from degrading permafrost to the atmosphere and its potential to degrade soil organic matter (especially carbon and nitrogen). Current understanding and knowledge of the microbial activity and its

metabolism in permafrost soils is very limited.
In this study, we propose a novel approach for monitoring biogeochemical activities in permafrost soils using microfluidic technology. The permafrost-on-a-chip contains soil, microbe, and all the minerals which enable the investigation of soil-microbe interaction. The freeze-thaw cycles of pore fluid are also considered. This microfluidic platform will be used to investigate the effect of freeze-thaw cycles on microbial activity and movement in the soil in real time (due to the transparent compounds that are used in designing the chips) by continuous monitoring of soil's moisture and temperature. The permafrost-on-a-chip technology is a significant step toward improving our comprehension of the processes that result in the emission of greenhouse gases and degradation of organic matter in permafrost soils around the world.

Participation:

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Energy Transition Focused Abstracts:

MS08 / **55**

Experimental and numerical investigation on convective mixing in porous media flows

Authors: Marco De Paoli[1]; Christopher Howland[1]; Roberto Verzicco[2]; Detlef Lohse[1]

[1] *Physics of Fluids Group, University of Twente*

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We use experiments and simulations to investigate the mixing dynamics of a convection-driven porous media flow. We consider a fully saturated homogenous and isotropic porous medium, in which the follow is driven by density differences induced by the presence of a solute. In particular, the fluid density is a linear function of the solute concentration. The configuration considered is representative of geological applications in which a solute is transported and dissolves as a result of a density-driven flow, such as in carbon sequestration in saline formations or water contamination processes. The mixing mechanism is made complex by the presence of the rocks (solid objects), which represent obstacles in the flow and make the solute to further spread, due to the continue change of the fluid path. Making predictions on the dynamics of this time-dependent system is crucial to provide reliable estimates of the evolution of subsurface flows and in determining the controlling parameters, e.g., the injection rate of a current of carbon dioxide or the spreading of a pollutant in underground formations. To model this process, we consider here an unstable and time-dependent configuration defined as Rayleigh-Taylor instability, where a heavy fluid (saturated with solute) initially sits on top of a lighter one (without solute). The fluids are fully miscible, and the mixing process is characterised by the interplay of diffusion and advection: initially diffusion controls the flow and is responsible for the initial mixing of solute. At a later stage, the action of gravity promotes the formation of instabilities, and efficient fluid mixing takes place over the entire domain. The competition between buoyancy and diffusion is measured by the Rayleigh-Darcy number (Ra), the value of which controls the entire dynamics of the flow. With the aid of experiments in

bead packs (optical measurements) and pore-resolved numerical simulations (immersed-boundary method), we analyse the time-dependent evolution of this system at high Ra, and we quantify the effect of the Rayleigh-Darcy number on solute transport and mixing. The results are analysed at two different flow scales: i) at the Darcy, where the buoyancy-driven plumes control the flow dynamics, and ii) at the pore-scale, where diffusion promotes inter-pore solute mixing. Numerical and experimental measurements are used to design simple physical models to describe the mixing state and the mixing length of the system. The results obtained are compared against previous experimental and numerical works.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS09 / **56**

Pore-scale simulation of hydrogen transport in porous media

Authors: Leila Hashemi[1]; Rainer Helmig[2]; Cornelis Vuik[1]; Hadi Hajibeygi[1]

[1] *TU Delft*

[2] *University of Stuttgart*

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Transition to renewable energy sources, due to their naturally intermittent production, requires developing large-scale storage technologies. Underground Hydrogen Storage (UHS) in porous formations is a promising approach to providing a giant storage capacity. To ensure the efficiency of the storage operation, multiscale modeling and simulation strategies are essential. Since micro-scale physics controls macro-behavior. Therefore studying the flow behavior in porous rocks at the micro-scale is insightful for UHS projects in porous reservoirs.
The present study develops a dynamic pore-network modeling (D-PNM) approach to simulate the immiscible two-phase flow of hydrogen and water through representative digital network models of different porous structures. As the key feature of UHS, the model is developed for the cycles of injection and production of hydrogen into a porous media. The model input parameters are based on the experimentally obtained static and dynamic wettability analyses as presented in the literature. As for the rock, digital networks are constructed based on 3D X-ray images of porous samples. The topology of the pore space geometry is translated to a representative pore-network model. To preserve the simulation stability, the developed D-PNM solves the transient multi-phase Stokes equations fully implicitly, for pressure and phase volume saturation. Through several test cases, we analyze the transport characteristics of the hydrogen/water interface, especially the fingering and spreading physics. These results shed new light on how a representative continuum-scale model should be created to study the process at the field scale.

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57

The influence mechanism of gas pressure on multi-scale dynamic apparent diffusion-permeability of coalbed methane

Authors: zhiqiang Li[1]; Lin Li[2]

[1] *Henan polytechnic university*

[2] *Henan Polytechnic University*

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The permeability and diffusion coefficient of the coal are the most important parameters affecting coalbed methane (CBM) extraction. There are multi-scale pores in coal with a huge difference in pore size. The permeability and diffusion coefficient of coal also show multi-scale characteristics due to the influence of multi-scale pore sizes. In the process of coalbed methane extraction, the gas pressure will continuously decrease. However, in current studies, there are contradictory perceptions of monotonically increasing, monotonically decreasing, and irregular fluctuations in the effect of gas pressure on diffusion coefficient and permeability. Therefore, it is essential to clarify the influence mechanism of gas pressure on multi-scale diffusion-seepage for CBM extraction. Diffusion-seepage experiments are carried out using 0.18~0.25 mm particle coal and Φ50 mm×100 mm cylindrical coal under different gas pressures and no stress loading. Meanwhile, seepage experiments measured by steady-state method are conducted using Φ50 mm×100 mm cylindrical coal under stress loading. The results show that the apparent diffusion coefficient attenuates dynamically with time in the experiments of particle and cylindrical coal without stress loading, and the classical diffusion model cannot accurately describe the full-time process of gas flow in coal. A model of multi-scale dynamic apparent diffusion is proposed, which can accurately depict the process of gas flow in cylindrical coal. The mechanism of gas flow in multi-scale pores is illustrated. At the beginning of the flow, gas first flows out of the large external pores. From the surface to the interior of coal, the pore sizes of gas flow gradually become smaller with increasing time, resulting in the gradual decay of the apparent diffusion coefficient. Based on the equivalent relationship between apparent diffusion coefficient and apparent permeability, the dynamic diffusion coefficient is converted into dynamic permeability attenuating with time. The initial apparent permeability decreases and then increases with the increase of gas pressure, which is caused by the effect of gas pressure stretching and multi-scale flow regime. The slip effect dominates in low gas pressure and stretching effect does in high gas pressure. The different changes of apparent permeability with gas pressure is related to a compressibility factor Ct. Three possible patterns of permeability with gas pressure, monotonically increasing, monotonically decreasing, and U-shaped will occur. The study reveals the influence mechanism of gas pressure on diffusion coefficient and permeability.

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Energy Transition Focused Abstracts:

MS10 / **59**

Characterization of oilwell cement with Ca-montmorillonite additives modified by supercritical CO2

Authors: Liwei Zhang[1]; KAIYUAN MEI[2]; Yan WANG[None]; Xiaowei Cheng[None]

[1] *Institute of Rock and Soil Mechanics, Chinese Academy of Sciences*

[2] *Institute of Rock and Soil Mechanics, CAS*

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High concentration CO2 invades oilwell cement under geological CO2 storage or sour oil and gas exploitation conditions. Long-term invasion of CO2 makes oilwell cement structure unstable and prone to damage. For the reinforcement of oilwell cement, Ca-montmorillonite (Ca-MMT) was modified using supercritical CO2 (ScCO2) as the solvent and intercalator. The micro-calcite bearing Ca-montmorillonite (MC Ca-MMT) was added to the cement slurry to reinforce the oilwell cement after the modification. Microcrystal calcite was identified in the MC Ca-MMT through transmission electron microscopy (TEM) and selected-area electron diffraction (SAED) analyses. The mechanical properties and microstructural evolution of the MC Ca-MMT reinforced oilwell cement were investigated, revealing that the carbonation was inhibited by MC Ca-MMT. Through the analysis of microcrystal formation and densified carbonation area, the CO2-resisting mechanisms of MC Ca-MMT reinforced oilwell cement were revealed in this study.

Participation:

In-Person

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MS03 / **60**

A New Upscaling Strategy for Flow in Fractured Porous Media

Authors: Daniel Stalder[1]; Daniel Meyer[2]; Patrick Jenny[None]

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[2] *Institute of Fluid Dynamics, ETH Zurich*

Corresponding Authors: jenny@ifd.mavt.ethz.ch, meyerda@ethz.ch, dstalder@student.ethz.ch

Given the high uncertainty of fracture characteristics in subsurface porous media, we focus in our work on the prediction of the mean or Ensemble Averaged Flow (EAF) field. Typically fractures can cover distances comparable to the size of the domain of interest. While classical homogenization only is valid for representative elementary volumes (REV) much larger than all embedded structures, the presented approach does not rely on such restrictions. The new model, which is formulated at this point for many isolated fractures, relies on a nonlocal multi-media description based on coupled integro-differential equations. It is shown how a previous description for fractures of equal length and aperture can be extended for much more realistic scenarios with multiple fracture families. With a series of numerical studies and comparisons with Monte Carlo reference data it is demonstrated that also for such more complex scenarios the devised sub-REV model accurately captures mean flow rates and pressure profiles for arbitrary domain sizes.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS03 / **61**

Visualising Two-Phase Flow in a Natural Geological Fracture Using Synchrotron Imaging

Authors: Tomos Phillips[1]; Tom Bultreys[2]; Kamaljit Singh[1]; van Stappen Jeroen[2]; Ben Callow[2]; Vladimir Bovak[3]; Christian Matthias Schlepuetz[3]; Stefanie Van Offenwert[2]; Veerle Cnudde[2]; Andreas Busch[1]

[1] *Heriot-Watt University*

[2] *Ghent University*

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Subsurface fluid flow primarily transpires in porous rocks, however, in low-permeability formations, interconnected rock fractures can govern fluid flow. Synonymous with fracture flow is the immiscible displacement of a wetting phase (e.g., brine) by a non-wetting phase (e.g., CO2), a process called drainage, which is fundamental to many subsurface engineering applications. Robust modelling of fracture drainage on the field scale is required to effectively predict and manage the risk of fault-related leakage. Despite this, the controls on leakage through a single fracture are only partially understood. Fluid transport through a natural fracture is complicated by aperture heterogeneity, which arises from opposing rough walls and the presence of discrete contact points related to chemical/stress alterations. For two-phase flow, phase interference is high in fractures as flow predominantly transpires in 2D rather than the 3D pore space of a rock matrix. Recent modelling and experimental studies have provided insight into how drainage progresses through fractured materials, however, a lack of investigation using a truly representative sample (natural rough fracture) at sufficient spatial and temporal resolutions limits the predictive insights of such studies. Here, we used fast synchrotron X-ray tomography to image drainage in a natural geological fracture (6 mm diameter & 18 mm length) obtained from the Carmel Formation, a regional caprock sequence overlying a naturally leaking CO2-charged reservoir in Green River, Utah (USA). Drainage was imaged continuously over ~3 hrs by capturing consecutive volumes at 2.75 μm voxel size with a 1 s scan time. The experiment was performed with analogue fluids (brine and decane) at a controlled fluid flux (capillary regime) analogous to that anticipated during CO2 fracture leakage. In this contribution, we will discuss the results obtained, which provide new insight into the micrometre-scale displacement processes that directly impact global fracture saturations (and leakage rates), and the key challenges associated with imaging drainage in such small fractures using synchrotron imaging.

Participation:

In-Person

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MS11 / **62**

Brine drying and salt precipitation in porous media: microfluidics quantification of pore heterogeneity and wettability impact

Authors: Hui Zhang[1]; Zhonghao Sun[2]; Nan Zhang[3]; Budi Zhao[1]

[1] *School of Civil Engineering, University College Dublin, Dublin, Ireland*

[2] *School of Human Settlements and Civil Engineering, Xi'an Jiaotong University, Xi'an, China*

[3] *School of Mechanical and Materials Engineering, University College Dublin, Dublin, Ireland*

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Deep saline aquifers are promising CO2 geological sequestration sites with wide distribution and large storage capacity. Pilot projects have shown that the injection of CO2 into saline aquifers can

lead to brine drying and salt precipitation, and eventually injectivity reduction. The interplay between gas injection, brine drying and salt precipitation determines the distribution of resulted salt crystals thus the impact on injectivity reduction. This dynamic process is influenced by rock properties (e.g., pore heterogeneity, surface wettability), initial salt concentration, gas injection rate, drying condition, etc. Laboratory experiments lead to inconsistent conclusions about these controlling factors, which indicates the lack of understanding of the mechanisms involved and hinders our prediction capability. Particularly, the pore heterogeneity and wettability of natural rock samples vary largely from site to site, and their impact on this dynamics process requires more detailed investigations. This study implements microfluidics to characterize pore-scale dynamics of brine drying and salt precipitation. We fabricate radial flow microfluidic chips with varying pore-space heterogeneity and surface wettability. A digital microscope records air invasion, brine drying and salt precipitation processes, while a pressure sensor monitors the injection pressure. We adopt a deep learning algorithm to automatically segment different phases, i.e., air, brine and salt crystals, in pore channels, which enables quantifying drying and precipitation rates and the evolution of brine clusters and salt crystals. Preliminary results indicate that pore heterogeneity determines the distribution of residual brine, i.e., increasing pore heterogeneity leads to more residual brine and salt precipitation. Also, the capillary backflow in hydrophobic chips significantly increases the accumulation of ions and salt precipitation near the drying front. In contrast, capillary backflow is absent after gas breakthrough in the hydrophobic chip, which results in the least amount of salt precipitation at the drying front. The quantitative results enable further statistical analyses on the evolution of brine cluster and salt crystals and their dependence on pore heterogeneity and surface wettability.

Participation:

In-Person

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MS14 / 63

Chemical and morphological uncertainty quantification by auto-weighted Bayesian Physics-Informed Neural Networks for reactive two-scale porous media at the pore scale

Authors: Sarah Perez[None]; Philippe Poncet[1]

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Data-driven approaches, among them machine learning tools, have garnered increasing interest in porous media research and offer alternatives to traditional numerical methods to improve the predictive modeling based on observation data. Recently, the idea of incorporating prior physical principles within measurements to better rely on experimental data has been successfully immersed into Bayesian inference as a valuable tool for uncertainty assessments.

The emergence of the Bayesian Physics-Informed Neural Networks (BPINNs) paradigm offers the opportunity to query the confidence in the predictions, the uncertainty in the measurements, and the model adequacy by providing posterior distribution of the neural network predictions [1]. In this presentation, we will show how to make BPINNs auto-weighted in order to address multi-objective IA problems, even when relying on shadow quantities.

Classical BPINNs mostly rely on Markov Chain Monte Carlo methods to sample from a weighted multi-objective target distribution, whose weights are related to the scaling of the tasks, the noise magnitude, and ultimately the inherent tasks'uncertainties. While these parameters are recognized as critical, they are mostly hand-tuned in the applications leading to pathological behaviours or biased estimation, in the sense that one of the objectives will be prevailing in the posterior distribution exploration.

Actually, when dealing with real-world complex systems which involve heterogeneities and multi-scale phenomena in addition to uncertainties in the measurements, the setting of these weights can remain particularly challenging and require considerable energy in tuning. Furthermore, such dynamics also raise scale imbalances that highly disrupt the usual approaches, generating instabilities that make the sampling inoperative.

We focus here on a novel adaptive strategy for unbiased uncertainty quantification in BPINNs, based on an inverse Dirichlet weighting [2] of the target posterior distribution, which remedies to the failure modes previously identified. Our approach provides enhanced convergence, stability, and balanced conditions between the different tasks which ensure an efficient exploration of the Pareto front throughout the sampling procedure. While reducing the bias in the sampling, we show that this strategy is able to automatically adjust the weights, with them the uncertainties, according to the sensitivity of each task.
It then offers an interesting framework to study complex multi-scale dynamics from the Bayesian inference perspective and incorporate uncertainty quantification in multi-objective and stiff inverse problems.

In this direction, we aim to capture and quantify unresolved features arising from noisy X-Ray micro tomography measurements by adding information on the predictive physical-chemical model and then compensate for the lack of knowledge on the rock matrix structure with PDE-based priors, established according to a Darcy-Brinkmann two-scale porosity model [3].
Hence, we apply our auto-weighted methodology to the simultaneous identification of chemical parameters and morphological uncertainties on the porosity field, in a reactive inverse problem at the pore scale.

Altogether with the approach developed in [4] to determine the absolute permeability deviation, we will be able to provide uncertainty quantification on the main macro properties of a porous media sample based on its micro tomography and then perform more relevant direct numerical simulations with respect to the experimental data.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS13 / **64**

Water diffusion in cellulose nanopores

Authors: Yuliang Zou[1]; Benjamin Maillet[2]; Philippe Coussot[3]

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Cellulose, the world's most abundant natural, renewable, biodegradable polymer, is a major component of plants, wood, paper, textiles or other industrial materials. A remarkable property of cellulose-based materials is that they can absorb huge amounts of water (typically 25% of the dry mass) from ambient vapor, in the form of bound water confined at a nanoscale in the amorphous regions of the cellulose structure. The control of the dynamics of sorption and desorption of bound water is a major stake for the reduction of energy consumption and material or structure damages. This dynamics relies on the ability of bound water to be transported through the material, but in the absence of direct observations this process is still poorly known. Here we present straightforward internal observations of bound water transport through a cellulose fiber piling filled with oil, which prevents vapor transport. Thanks to NMR relaxometry and MRI measurements we show that the bound water is transported along the fibers and throughout the network of fibers in contact. This process may be well described by a constant diffusion coefficient. The dependence of this diffusion coefficient on the fiber density and orientation is then analyzed to deduce the (elementary) diffusion coefficient of bound water along a cellulose fiber axis. Surprisingly, although the bound water molecules are confined in nanometric pores between cellulose microfibrils, the diffusion coefficient is in the order of the coefficient of self-diffusion of water. This constitutes fundamental physical data which may be compared with molecular simulations, and opens the way to the prediction and control of sorption dynamics of all cellulosic materials or other hygroscopic materials.

Participation:

In-Person

References:

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Poster / 65

Performance characterization of oil-based drilling-mud contaminated cement as a barrier material

Authors: Elie Ngouamba[1]; Benjamin Maillet[2]; Rahima SIDI-BOULENOUAR[None]; Philippe Coussot[2]; Nils Opedal[3]

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Cement plug is a crucial barrier material for ensuring long-term integrity of depleted wells, either where CO2 has been sequestered or in permanently abandoned wells [1]. However, some of the drilling mud used prior to the cementing operation often remain due to wetting properties of the base mud [2]. The remaining drilling mud might therefore contaminate the cement and can be detrimental to permanent plugging and abandonment as it might not only affect the intrinsic properties of the cement (mechanical strength, porosity, permeability) but also the properties of the cement-casing interface (bonding, hydraulic sealing). Eventually this can induce leakage paths such as microannuli (crack between cement and casing).

In this study, we investigate the effect of oil-based drilling mud (OBDM) contamination on the sealing properties of cement and cement-casing interface, on a macroscopic and a mesoscopic scale.

Different fractions of OBDM are dispersed in a neat Portland G cement. First, the mechanical properties of contaminated cements are monitored under relevant downhole conditions, high pressure and high temperature (HPHT): in the liquid state we used a rheometer with a HPHT cell to evaluate the slurries flow properties and an ultrasound cement analyser (UCA) to assess the setting time. In the hardened state we used the UCA, to monitor cement strength. The compressive strength of the cement tends to decrease with the OBM contamination, while the viscosity increases significantly indicating a deterioration in its pumpability.

Secondly a tailor-built plug integrity experimental set-up [3], which allows us to simulate cement placement and curing, and to assess plug integrity by inducing a differential pressure and monitoring the resulting flow rate, is used to assess the overall integrity of the contaminated cement and casing through their effective permeability.

Finally at the mesoscale we used nuclear magnetic resonance (NMR) [4] to follow oil phase evolution during cement hardening and analyse the relationship with the resulting macroscopic properties of the contaminated cement.

Participation:

In-Person

References:

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MS13 / **66**

The phase equilibria of aqueous electrolytes in confinement under Martian condition

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The discovery of chlorides and perchlorates has profoundly influenced our view of liquid water on Mars [1,2]. These salts attract much attention, because their hygroscopic nature and low eutectic temperature allow for the possibility of liquid water on the surface of Mars today. Recent studies showed the confined space exert significant effect on the phase boundary on salt solution, particular in the freezing and deliquescent process [3,4].

In this work, we perform experiments to investigate the eutectic temperature and deliquescence humidity of Mars-relevant salts (CaCl2, MgCl2, Ca(ClO4)2, and Mg(ClO4)2) in bulk and various size pores (3–20 nm). The results indicate that, compared with water, the confinement effect on melting temperature of salt solutions is more significant. It was found that freezing of concentrated solutions in narrow pores can even be suppressed completely. The deliquescence humidity of salts in pores is much lower than bulk particle, and the hydration dynamic process may be influenced for the deliquescence humidity shift. In order to understand the salt and confinement effects on the stability field of a liquid water phase, we develop an ion interaction model (based on Pitzer theory) to calculate the phase diagram of cryogenic aqueous solutions.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / **67**

Experimental study of the sealing properties of cement plug during the early age

Authors: Nils Opedal[1]; Even Wiggen[2]; Elie Ngouamba[2]; Ragnhild Skorpa[2]

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In sequestered CO2 underground wells or in permanently abandoned wells, a cement plug is typically used as a well barrier material to ensure long-term zonal isolation of the well [1]. Proper plugging should prevent any flow of fluids from the well to the surrounding environment and the surface. It is assumed that the ability of the cement plug to fulfil its barrier function over the long term depends on its behaviour from the early age to the hardened state [2]. A good knowledge of this initial stage might allow prediction of potential crack (microannuli) formation between the cement and casing. In this study we investigate the impact of curing time during the early age of the cement plug, on its sealing properties in a scaled-down configuration but under relevant downhole conditions.

In the first stage we use an Ultrasonic Cement Analyzer (UCA) to monitor the evolution of cement strength over time, under appropriate downhole conditions. From this test, we mainly detect 3 phases: before the setting time (zero and no cement strength), a second phase where we have a strong increase of cement strength (transient state) and a third phase where the cement strength increase is negligible (steady). This allows us to select times we use as curing times before performing a plug integrity test in the transient and steady states.

In the second stage, we use a custom-built set-up [3] with which we simulate and evaluate the integrity of the plug by inducing several differential pressures and monitoring the resulting flow rates. The cement slurry is always identically mixed and placed but cured for different durations. The slope of the curve of flow rate as a function of differential pressure, namely the effective permeability of the cement-casing system falls in two distinct regions.
For curing time in the steady state, the neat Portland G cement exhibits a rapid gas breakthrough and relatively high flow rates compared to the time in the transient state. However, for curing time in the transient state, the pressure breakthrough of the gas is delayed, and the flow rates are very low or almost not observed. This suggests a degradation of the bondings and thus
of the sealing properties of cement with time despite the significant increase in cement strength.

Participation:

In-Person

References:

[1] T. Vrålstad, A. Saasen, E. Fjær.; T. Øia, J.D. Ytrehus; M. Khalifeh, Plug & abandonment of offshore wells: Ensuring long-term well integrity and cost efficiency, J. Pet. Sci. Eng. 173 (2019), 478–491.

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68

Experimental study on methane hydrate formation and decomposition characteristics in a micromodel

Authors: Jianbo Zhang[None]; Jihao Pei[None]; Xiaohui Sun[None]; Bangtang Yin[None]; Baojiang Sun[None]; Zhiyuan Wang[None]

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This work carried out methane hydrate formation and decomposition experiment under gas-water flow conditions in a micromodel. The micro experimental facility for methane hydrate methane hydrate formation and decomposition were set up, which mainly includes gas source, etched micromodel, gas and water storage tanks, refrigeration system, water injection pump, CCD camera, data monitoring system, back pressure pump, gas-water separation device, gas flowmeter, pressure reducing valve, and various control valves, etc. During the experiments, the hydrate formation, deposition, plugging and decomposition processes in the pore channels of the etched micromodel can be clearly observed and amplified, which was used to analyze the characteristics of hydrate formation and decomposition. In addition, the effect of pressure on hydrate formation and decomposition was also experimentally studied.

The experimental results show that the hydrate formation and deposition rates varied in different pore channels, and the hydrates formed in the pores tended to be deposited in situ. The hydrate fraction at the intersection of different channels was significantly higher than that of a single channel, increasing the risk of hydrate plugging in pore channels. Hydrate plugs may contain some free water or methane gas that does not completely form the hydrate. The variation in the hydrate fraction in the pores has stages of rapid growth, slow growth, and dissolution. Meanwhile, owing to the difference in the gas–water flow distribution caused by hydrate plugging, the hydrate plugging time at different pore channels follows a certain order. The higher the pressure, the more likely hydrate plugging will occur. Once the pressure at the outlet of the micromodel model decreases, the hydrate in the pore channel starts to decompose into methane gas and water. It is suggested that the decomposition of hydrate gradually advances from the outlet end to the inlet end, which was mainly affected by the pressure transmission. The methane gas generated by hydrate decomposition exists in two forms: one is the continuous phase that forms the gas flow channel, the other is the gas bubbles dispersed in water. The greater the pressure drop at the outlet, the faster the hydrate decomposition rate. This work can provide valuable experimental foundation for hydrate formation and decomposition prediction models in porous media.

Participation:

Online

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Energy Transition Focused Abstracts:

MS08 / 71

Quantification of the impact of acidified brine on fracture-matrix transport in a naturally fractured shale using in situ imaging and modeling

Authors: Christopher Zahasky[1]; Manju Pharkavi Murugesu[2]; Takeshi Kurotori[3]; Collin Sutton[1]; Jennifer Druhan[None]; Bolivia Vega[None]; Sally Benson[2]; Anthony Kovscek[2]

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[2] *Stanford University*

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Understanding flow, transport, chemical reactions, and hydro-mechanical processes in fractured geologic materials is key for optimizing a range of subsurface processes including carbon dioxide and hydrogen storage, unconventional energy resource extraction, and geothermal energy recovery. Flow and transport processes in naturally fractured shale rocks have been challenging to characterize due to experimental complexity and the multiscale nature of quantifying exchange between micrometer-scale fractures and nanometer-scale pores. In this study, we use positron emission tomography (PET) to image the transport of a conservative tracer in a naturally fractured Wolfcamp shale core before and after exposure of the core to low pH brine conditions. Image-based experimental observations are interpreted by fitting an analytical transport model to every fracture-containing voxel in the core. Results of this analysis indicate subtle increases in matrix diffusivity and a strong reduction in fracture dispersivity following exposure to low pH conditions. These observations are supported by a multi-component reactive transport model that indicates the capacity for a 10% increase in porosity at the fracture-matrix interface over the duration of the low pH brine injection experiment. This porosity enhancement is the result of exposure of carbonate minerals in the shale matrix to low pH conditions. This workflow represents a new direct approach for quantifying fracture-matrix transport processes and provides a foundation for future work to better understand the role of coupled transport, reaction, and mechanical processes in naturally fractured rocks.

Participation:

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References:

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72

Pore network extraction from multiscale images: an efficient approach based on artificial neural network

Authors: Abolfazl Moslemipour[1]; Saeid Sadeghnejad[1]

Co-authors: Javad Razavi Nezhad [1]; Davood Khoozan [1]; Frieder Enzmann [2]; Michael Kersten [2]

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More than half of the world's oil is reserved in heterogeneous carbonate and tight sandstone rocks. A comprehensive understanding of rock properties is essential for efficient production from these reservoirs. Digital rock physics (DRP) is an approach that has been used in recent years to evaluate rock properties on the pore scale. Image acquisition techniques by industrial/synchrotron X-ray CT, FIB-SEM, etc., are the primary source of data for DRP. Heterogeneous rocks with porosities at various scales are mostly imaged at multi-scales because of the trade-off between the resolution and field of view (FoV) [1, 2]. One of the most crucial prerequisites for DRP is the correct pore network

extraction from images with methods such as SNOW [3] or Maximal ball [4]. However, the extraction of pore network models (PNMs) from multi-scale images is limited due to high computational costs and high memory demand for the tremendous number of pixels/voxels in rock images. For this reason, PNMs are usually extracted on a smaller FoV, which makes it impossible to represent the heterogeneity in rocks. Therefore, it is vital to develop an approach to extract PNMs from multi-scale images with a higher speed and less memory usage while maintaining accuracy.
This paper aimed to introduce an efficient PNM extraction method from images at multiple resolutions. The conventional method to increase the extracted network accuracy is to use an image with the highest resolution, which is memory demanding and has the highest computational cost. We introduce a novel rock image with variable voxel sizes to solve this problem. The basis of this approach is the separation of the resolved and unresolved porosities with different voxel sizes. The unresolved porosities are subdivided into smaller regions using the marker-based watershed algorithm [5]. These regions are then replaced with image templates extracted from the higher-resolution image. The result is a multi-resolution image with dual-voxel size, i.e., large and small voxels for resolved and unresolved regions. The SNOW algorithm is then used to extract pore networks from both regions separately. Finally, an artificial neural network (ANN) trained on the high-resolution image is implemented to link both networks together. The unresolved networks are first connected to each other and then are connected to networks extracted from resolved regions. The synchrotron CT images of a Berea sandstone rock at multiple resolutions are used as our training dataset. The results show an excellent agreement between the porosity and permeability (computed by the OpenPNM library [6]) of the extracted multi-scale PNM and that of the high-resolution images. The suggested approach is also considerably faster in extracting the PNM than the SNOW and Maximal Ball methods applied directly to the high-resolution image.

Participation:

Online

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Image resampling: a vital prerequisite step in multi-scale modelling of heterogeneous rock samples

Authors: Abolfazl Moslemipour[1]; Saeid Sadeghnejad[1]

Co-authors: Javad Razavi Nezhad [1]; Davood Khoozan [1]; Frieder Enzmann [2]; Michael Kersten [2]

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Resampling is an interpolation technique that is used to increase (upsampling) or decrease (downsampling) the resolution of images by the desired ratio. Upsampling or downsampling and changing the resolution of images to fuse them with different resolutions is one of the most important applications of resampling methods in the digital rock physics (DRP) workflow [1-4]. The resampling approach is mostly applied to images of heterogeneous rocks because of the existence of pores at various scales. In these rocks, due to the trade-off between resolution and field of view, it is not possible to obtain fine and coarse scale properties using a single image and images at multi-scales must often be fused. Therefore, there is a greater need for resampling methods in the multiscale modelling of these heterogeneous rocks. There are various methods available in the literature for image resampling. It is crucial to choose an appropriate resampling method to avoid image property alteration during this process.

In this paper, we first applied three different resampling methods (Lanczos [5], Bi-Linear [6] and Bi-Cubic [7]) on the images of two rocks: a Berea sandstone and a carbonate rock sample. Avizo (Thermo Fisher Scientific) was used to apply the resampling process on the images, and Python codes and libraries were used to compute their properties. To determine the resampling impact on image properties, we repeated this process on a range of scales with various coefficients. We calculated the geometrical and flow properties of the resampled images by all three methods. The rock properties include porosity, permeability (computed by OpenPNM [8]), Euler number (computed by an in-house Python code), and capillary pressure curve (OpenPNM [8]). The properties of the original image were compared with that of the resampled images. Based on the results, the sensitivity of carbonate rock properties to resampling was higher than that of sandstone. Moreover, the Bi-Cubic method showed the least change in both rock properties. For permeability, both Lanczos and Bi Linear methods showed almost the same results (Lanczos was slightly better), but the Bi Linear method was less sensitive to the other properties. Moreover, resampling (both downsampling and upsampling) by more than 5% in carbonates and by more than 6% in sandstones will drastically alter the above-mentioned properties, which will produce unrealistic results.

Participation:

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Quantitative evaluation of microscopic distribution morphology and saturation calculation of natural gas hydrate

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Natural gas hydrate is a potential alternative energy sources in the future, with large resource reserves, wide distribution regional and high combustion calorific value. Electrical properties as one of the most important physical characteristics of gas hydrate-bearing sediments, which are considered as the key parameters for gas hydrate well logging identification, saturation calculation and reserve estimation. However, there are three main pore-habits for gas hydrate in sediments, i.e. pore-filling, cementing, grain-coating, which have a significant effect on the resistivity of gas hydrate-bearing sediments. Besides, there is a close relationship between gas hydrate saturation and gas hydrate pore-habits. Hence, it is of great significance to explore the influence of gas hydrate pore-habits and saturation on the resistivity, and to propose a new calculation model for gas hydrate saturation. This research combines the experimental method of gas hydrate formation and the finite element method to improve the understanding of relationship between resistivity and gas hydrate pore-habits and saturation. We utilized high-resolutions X-ray CT technology to observe the gas hydrate formation process in sand sediments, and obtained the quantitative data of different pore-habits of gas hydrate. Then, found the inflection point of the proportion of different pore-habits of gas hydrate through data analysis. Besides, extracted and built the digital gas hydrate sediments models, containing the pore structure and gas hydrate distribution information. Then, we implemented the experimental models in an electrical-properties simulation program to calculate resistivity. Through analyzing the calculated results, it was feasible to explain the variations of pore-habits in gas hydrate formation process, and clarify how the gas hydrate's pore habits influences the relationship between resistivity and hydrate saturation in hydrate-bearing sediments. Finally, we segmentation fitting of the relationship between gas hydrate saturation and the saturation index in Archie's formula, and proposed a new calculation model of gas hydrate saturation. The practical application results show that the new model has good accuracy and reliability.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

75

Pore-Scale Modelling on Hydrogen Transport in Porous Media: Implications for Hydrogen Storage in Saline Aquifers

Author: Jinlei Wang[1]

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[1] *China University of Petroleum (East China)*

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Hydrogen energy has tremendous potential as a clean fuel in this energy transition. To build up the full-scale hydrogen energy supply chain, large-scale hydrogen storage is of vital importance. Underground hydrogen storage in saline aquifers has been perceived as an important means to achieve large-scale hydrogen storage. Therefore, we investigated hydrogen transport in pore network in a sandstone porous media at strongly water-wet and weakly water-wet (hydrogen- wet). We performed direct numerical simulation through volume of fluid method to investigate the transport of hydrogen at pore-scale under different wetting conditions with input hydrogen-rock physics data from literature.

Our results showed that during primary drainage process (hydrogen injection for storage purpose), increasing hydrogen wetting decreased snap-off effect, enabling a greater pore space for hydrogen storage. During primary imbibition process (hydrogen extraction), increasing hydrogen wetting promoted the size and stability of hydrogen clusters, which is unfavorable to hydrogen extraction process. Given the significant high interfacial tension between brine and hydrogen and low viscous force of hydrogen, snap-off effect dominates the flow in both hydrogen injection and extraction process regardless of wetting conditions. This physical process causes the recovery factor even below 20%. We therefore suggest that storing hydrogen in depleted gas reservoirs under irreducible water saturation would have much less risks in hydrogen trapping during extraction process.

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Poster / 77

Spatial moment analysis of single-species transport in unidirectional laboratory tracer tests using rock cores

Authors: Amarjot Singh Bhullar[1]; Riccardo Standish[1]; Ronny Pini[1]

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In the study of solute transport in porous media, it is common to rely on the Advection Dispersion Equation (ADE) model to interpret effluent breakthrough curves (BTCs) post unidirectional tracer laboratory tests. However, this approach is not suitable for porous rocks, as these are characterised by transport processes that occur over a wide range of length- and temporal scales. To deliver better subsurface engineering solutions in complex porous media, whether it be for groundwater contaminant tracking, carbon capture and storage (CCS), or geothermal/petroleum resource extraction, a workflow that integrates an updated experimental approach, and a novel means of data processing is necessitated.

Here, we deploy a numerical optimisation routine to fit experimental BTC data measured on Bentheimer Sandstone (BS), Ketton Limestone (KL), and Edwards Brown Carbonate (EB), at different flowrates and published previously (Kurotori et al. 2020). Although we use the ADE model to fit the BTC data of BS (a homogeneous sandstone), the Multi-Rate Mass Transfer (MRMT) model was used to fit the BTC data of KL and EB, two highly heterogenous carbonates. The analysis includes the estimation of parameters' uncertainty by Bayesian inference. These parameter values (and their uncertainties) are then used to evaluate the first four spatial moments of the internal concentration distribution, representing the temporal evolution of total mass (0th), centre of mass (1st), variance (2nd), skewness (3rd) and kurtosis (4th). Unique to this study, the predicted moments are compared to their experimental counterparts, which have been estimated from 4D solute concentration measurements obtained by Positron Emission Tomography (PET) imaging.

We demonstrate that PET can be used to precisely measure the spatial moments of the solute concentration and that these present unique features depending on the rock type. We show that for BS the spatial moments are insensitive to flow rate when plotted as a function of pore volumes injected (PVI). However, for the two carbonate rocks, they feature a flow rate dependency, due to the presence of microporosity and vugs, which introduce porous regions of virtually stagnant flow - where transport is largely dominated by diffusion. For the two carbonate samples, both 0th and 1st moment yield earlier breakthrough, and greater tailing of the solute mass with increasing flowrate. The

2nd moment takes much larger values for KL and EB than BS, indicating greater spreading of the tracer pulse and less mixing due to the larger contrasts in activity between the immobile and mobile zones. This is further exacerbated at higher flowrates. For BS, the 3rd and 4th moments prior to breakthrough take constant values at 0 and 3, respectively, indicating that the tracer plume is normally distributed. Yet, lower values are observed for the carbonates, reflecting an evolving skewness of the tracer plume during transport.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / **78**

Mineral Dissolution on Geological Carbon Storage in Carbonates: A Microcalorimetric Study

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Carbon capture and storage (CCS) is a key technology to reduce CO2 emissions and reach long term climate goals, aiming to limit the temperature rise to 1.5 ◦C above pre-industrial levels. CCS consists of capturing CO2 from large industrial processes or from burning fossil fuels in power generation. The captured CO2 is thereafter transported via pipelines or ships and stored in appropriate geological formations, such as depleted oil and gas reservoirs, unminable coal beds, and deep saline aquifers [1]. The existence of infrastructure, the wealth of reservoir data, and revenue from incremental oil recovery make depleted oil and gas reservoirs the best option for underground CO2 storage [2]. Carbonate reservoirs may be candidates for CO2 sequestration through CO2-EOR since those reservoirs hold more than 50% of the known petroleum reserves worldwide [3]. The main issue with CO2 injection into carbonate reservoirs is the formation of carbonic acid that ionizes to form hydrogen ions and bicarbonate ions. This weak acidic environment could alter the performance of carbonate CO2 storage reservoirs due to dissolution processes that lead to the formation of highly porous and conductive wormholes [4].

Long-term CO2 sequestration in carbonate reservoirs requires comprehensive assessments of CO2-reservoir fluid-mineral interactions. However, this is not an easy task due to the complexity of the

reservoir
fluid and rock-forming minerals. In the present work, the interfacial-phenomena at rock-aqueous interface during CO2 injection in carbonate rocks is evaluated by a highly sensitive microcalorimetry technique called that is Isothermal titration calorimetry (ITC). Cobos et al. [5] reported that accurate adsorption enthalpy values for complex rock-fluid systems can be obtained by microcalorimetry. In the ITC experiments, 100 mg of Edwards limestone powder (< 100 µg) was placed in a reaction vessel and 200µL of North Sea formation brine (NFB) was added to the particles. The titration ampule containing the rock-brine slurry was lowered step by step into the calorimeter and equilibrated for 1 hour at 40 ◦C. Seven injections of 9.948 µL of 3.5 wt% NaCl brine saturated with CO2 (BCO2) were injected independently into the limestone+NFB system with an interval time of 420 seconds between injections. Fluid-fluid experiments consisted in injecting BCO2 into NFB. Baseline rock-fluid-fluid and fluid-fluid tests were performed similarly but without CO2.

This work shows that dynamic rock–fluid and fluid–fluid interactions take place upon CO2 injection into carbonate rocks due to composition variation "waves"that alters the equilibrium in the system. The results from the Isothermal Titration Calorimetry (ITC) indicate that the dissolution process due to the formation of a weak acidic environment is driven by entropy. This dissolution process is unfavorable with respect to enthalpy change but thermodynamically favorable with respect to entropy change (increment of cations and hydrogen carbonate in the brine). A large perturbation in the water-water network was observed when BCO2 was injected into the reservoir fluid. This alteration is a result of the salinity difference and also the presence of CO2 in the injection fluid.

Participation:

In-Person

References:

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MS11 / **79**

Nanofluidics: a window into pore-scale fundamentals of CO2 in-

jection in shale

Author: Junjie Zhong[1]

[1] *China University of Petroleum (East China)*

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Shale resources are massive, controversial, and provide an increasing share of global energy with a broad group of stakeholders in academia, industry, and government. CO2 injection is promising for enhancing shale resource recovery due to its high mobility in tight porous media and strong extraction capacity for hydrocarbons. Meanwhile, the injected CO2 can be sequestered in the reservoir to achieve the carbon neutralization goal. The shale reservoir is featured by its nanometer pores. Due to the unique nanoscale confinement effect, the interactions among CO2, reservoir fluids, and minerals in shale differ from that in conventional reservoirs.

In this presentation, we would like to introduce our recent nanofluidic and theoretical work in investigating nanometer pore-scale CO2 injection fundamentals. Emergent topics include nanoconfined CO2-oil miscibility and CO2-induced salt precipitations. The nanofluidic experiments indicate deviations from classical theory predictions, due to the multiscale nature of the shale matrix. The miscibility between CO2 and oil at the nanoscale is found to shift from the bulk value and varies with pore structures. The salt precipitation and dissolution rate during the CO2 injection is slowed by orders of magnitude from theoretical predictions. In addition, the nanofluidic device has also been applied to characterize the phase behaviors of gas condensate at the nanoscale. The upper dew point is measured to deviate from the bulk value significantly, and is affected by pore size distributions. We see massive opportunities in leveraging nanofluidic devices to evaluate relevant fluid phases and transport fundamentals of CO2 injection in shale. The experimental findings can provide solid support for theoretical modeling and simulation.

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Energy Transition Focused Abstracts:

80

Pore-scale modeling using 3D electron tomography data of the cathode catalyst layer of a PEM fuel cell

Authors: Supriya Bhaskaran[None]; Nicole Vorhauer[1]; Jasna Jankovic[2]

Co-authors: Tanja Vidaković-Koch [3]; Evangelos Tsotsas ; Vikranth Kumar Surasani [4]

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The study of the structural parameters of the cathode catalyst layer (CL) of Polymer Electrolyte Membrane (PEM) fuel cells is a crucial step for pore-scale modeling and the base for understanding the coupling of two-phase transport processes with reaction. Of major interest is the location of active catalyst sites. The reaction occurs at carbon-supported platinum nanoparticles satisfying a condition of a so-called three-phase boundary. At the three-phase boundary, oxygen saturated ionomer phase is in contact with platinum nanoparticles and gas-transporting void space. Having an actual 3D model of the CL obtained by imaging is crucial to develop a realistic pore-scale model.
For this purpose, the cathode CL nanostructure of a commercial membrane electrode assembly (MEA) was imaged using the electron tomography TEM technique. The measurements were conducted with a source voltage of 200kV and a current of 2 nA. The scanned sample had an approximate total volume of 500 × 500 × 100 nm3. From this, a 3D domain of 138 × 138 × 58 nm3 was reconstructed for this study.
From the image data, the different phases (void fraction, carbon, ionomer, Pt-particles) are identified using Avizo segmentation Editor and ImageJ tools. The aim of this study is to identify the connectivity of ionomer within the CL and with the membrane, as well as carbon and pore space with the gas diffusion layer. While the ionomer connectivity is mandatory for the transport of H+ ions, the carbon mediates the electron (e-) transport, and the feedstock oxygen is transported through interconnected pores (Fig. 1). The limits of the connectivity and the degree of utilization are of major interest in this study. This concerns especially the noble metal platinum, for which the loading of the CL should be principally reduced to a minimum. The structural information shall then later be used as input data for pore-scale models (Lattice Boltzmann and pore network models), where the active platinum particles will be assigned as reactive catalytic sites.

Fig. 1 a) Reconstructed image of the CL. b) Schematic representation of the cathode catalyst layer: The ionomer is represented in blue; the carbon for electron connectivity is represented in black; pore space for O2 transport in white; the red circles represent the active sites, i.e., Pt-particles located at the three-phase boundary of ionomer, carbon and oxygen-filled pore; the yellow circles represent the inactive sites, i.e., Pt-particles that are not located at the three-phase boundary.

Participation:

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MS22 / 81

Diffusion properties of the gas diffusion layer from three dimensional digital images of the fibrous substrate and the microporous

layer

Authors: Mohamed El Moustafa AHMED MALOUM[1]; Thomas DAVID[2]; Laure GUETAZ[2]; Paul DURU[3]; Joël PAUCHET[2]; Michel QUINTARD[4]; Marc PRAT[3]

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inp.fr, thomas.david3@cea.fr, michel.quintard@toulouse-inp.fr

Direct numerical simulations are performed on reconstructed two-scale three-dimensional digital images in order to compute the effective diffusion properties of a gas diffusion layer (GDL) made of the assembly of a fibrous gas diffusion medium (GDM) and a microporous layer (MPL). The two-scale digital images are obtained by using micro X-ray computed tomography for the microporous GDM microstructure and MPL cracks, and focused ion beam-scanning electron microscopy (FIB-SEM) for the nanoporous MPL matrix. The MPL matrix effective diffusion tensor is first computed from the FIB-SEM reconstructed 3D images considering Knudsen and Fickian diffusions. Then the GDM-MPL assembly effective through-plane diffusion coefficient is computed thanks to a mixed approach combining a continuum description for the MPL matrix and the explicit discretization of the MPL cracks and GDM pore space. The impact of MPL cracks on the assembly diffusion properties is evaluated by comparison with the case without cracks. The impact of the MPL penetration into the GDM and the impact of the GDM compressibility are evaluated using a diffusive resistance model, validated from the numerical simulations.

Participation:

In-Person

References:

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MS03 / 82

Modeling Matrix-Fracture Fluid Leakage in Fractured Rocks Using Multi-Scale Darcy-Brinkman-Stokes Approach

Authors: Xupeng He[1]; Zhen Zhang[1]; Yiteng Li[1]; Marwa AlSinan[2]; Hyung Kwak[2]; Hussein Hoteit[3]

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Objectives/Scope
Understanding the fundamental mechanisms of fracture-matrix fluid exchange is crucial for the modeling of fractured reservoirs. Traditionally, high-resolution simulations for flow in fractures often neglect the effect of matrix contribution on the fracture hydraulic behavior. In this study, we develop a multi-scale approach to capture the matrix-fracture leakage interaction and its impact on the hydraulic properties of roughed fractures.

Methods, Procedures, Process
Because of the multiscale nature of the fracture and matrix rocks, full physics Navier-Stokes (NS) simulation in both matrix and fracture media is not feasible. For such multiscale phenomena, we use NS equations to describe the flow in the fracture, and Darcy's law to model the flow in the surrounding porous rocks. The hybrid modeling is achieved using the extended Darcy-Brinkman-Stokes (DBS) equation. With this approach, a unified conservation equation for flow in both media is applied. We use an accurate Mixed Finite Element approach to solve the extended DBS equation. Analytical solutions were used to verify the numerical method.

Results, Observations, Conclusions
Various sensitivity analyses were conducted to explore the leakage effects on the hydraulic aperture of rock fractures by varying the permeability of the surrounding medium, fracture roughness, and Reynolds number (Re). A series of pore-scale simulations for flow through roughed fractures were performed, and the results were used to develop a relationship between the flow rate and pressure loss. Streamline profiles show the presence of back-flow phenomena, where in- and out-flow are possible between the matrix and the fractures. Further, zones of stagnant (eddy) flow are observed within locations of large asperities of sharp roughness within the fracture and high Re. This implies the presence of dynamic trapping mechanisms that may impact the relative permeabilities and residual saturations within the fractures. Numerical results show the side-leakage effect can create non-uniform flow distribution in the fracture that deviates significantly from the flow with impermeable wall conditions. The proposed friction factor has the potential to be used as an upscaling tool to estimate the hydraulic properties of roughed fractures within permeable rocks in fractured reservoir simulations.

Novel/Additive Information
We develop a high-resolution approach to investigate the flow exchange behavior between the fracture and rock matrix. We investigate static and dynamic effects, including variable Reynold numbers, mimicking flow near and away from the wellbore. We show that local fracture characteristics such as roughness and tortuosity may impact the flow, which is often not accounted for in dual-porosity simulations. We propose a new upscaling friction factor to account for these mechanisms in field-scale reservoir simulations.

Participation:

In-Person

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Poster / 83

Thermoregulation and Ventilation in Termite Nests: Towards Bio-Inspired Solutions to Design Energy Efficient Buildings

Author: Nengi Fiona Karibi-Botoye[1]

Co-authors: Guy Theraulaz [2]; Vasily Demyanov [1]; Bagus P. Muljadi [3]; Athanasios Nathanail [1]; Hannah Menke [1]; Julien Maes [1]; Kamaljit Singh [1]

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[2] *Centre de Recherches sur la Cognition Animale (CRCA), Centre de Biologie Intégrative (CBI), Université de Toulouse,CNRS, UPS, Toulouse, France.*

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Abstract
Termite nests have long been recognised for their ability to maintain self-sustained ventilation and thermoregulation irrespective of external climatic conditions. Although there has been significant interest in this topic, especially from a point of view of designing energy-efficient buildings, the mechanisms by which the nest properties are controlled are not fully understood.
In this study, we investigate how the structural properties of termite nests, constructed by different termite species, affect temperature regulation and ventilation. We combine X-ray tomography, numerical simulations, and machine learning to correlate nest properties with climatic conditions. The results show that termite nests in the savannah vegetation have similar architecture and structural properties and have larger surface to volume ratio and surface complexity compared to nest in the forest vegetation. Large surface to volume ratio and surface complexity are properties which have been linked to efficient gas exchange and reduced nest insulation. The results will be correlated to pressure and velocity fields, permeability, thermal conductivity, and CO2 dispersivity obtained from millimetre-scale 3D numerical simulations, which will enable us to better understand the processes that control self-sustained ventilation and thermoregulation in termite nests.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS11 / 85

Investigation of Nanogel Transport in Porous Media by Microfluidic Models

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Polymer nanogels, crosslinked polymer particles, have attracted increasing interest in Enhanced Oil Recovery (EOR) field. However, it is still unclear that how to properly utilize nanogels to reach their full potential in oilfields because the transport mechanisms of nanogels in porous media are not well understood so far. In this work, we synthesized a fluorescent nanogel and visualized the transport and retention of fluorescent nanogel in 3D transparent glass micromodels that are manufactured by packing glass beads in capillaries. Finding the relationship between fluorescent intensity and nanogel concentration, we quantified transport velocity, concentration distribution and corresponding pressure gradient by confocal microscopy.
It was found that in a micromodel with a permeability of around 6 Darcy, these elastic polymer particles could transport at a pressure gradient of about 2 psi/ft. Besides, we proposed a new method to calculate dynamic adsorption of nanogel in porous media and showed the influence of flow rate on adsorption thickness. The results showed that the adsorption decreased with increasing flow rate and the adsorption density was about 6mg/g with the adsorption thickness of 1-2μm. We also found that the transport of polymer nanogels followed convection diffusion equation very well. This research improved the understanding of polymer particle transport in porous media and provided a novel method to obtain the kinetics of dynamic adsorption.

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In-Person

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A Productivity Analysis Method Of Low Permeability Reservoir In Beibuwan Basin

Author: Lei Wang[1]

Co-authors: Wenjuan Wang [2]; Qiaoliang Zhang [2]; Guangqing Yao [3]; Shaofei Yue [2]

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The test productivity of offshore reservoirs with low permeability are obviously different from the actual productivity in Beibuwan (BBW) Basin, western South China Sea. It is caused by the short testing time of the exploration wells. To solve the problem, a productivity analysis method is established based on the generalized Darcy formula and the conservation of mass. The factors are considered in the method and effectively quantified for the effect on productivity, including non-Darcy seepage of low-speed, stress sensitivity and maintenance level of formation pressure. Through fitting non-Darcy seepage experimental data of water flooding in 45 core samples from BBW Basin by different seepage formulas, the generalized Darcy formula considered effective driving coefficient can characterize non-Darcy seepage. The equations of productivity prediction for oil-water flow are established based on the conservation of mass. According to the influencing analysis of non-Darcy seepage of low-speed and stress sensitivity on productivity in the low-permeability reservoir of BBW Basin, the results indicated that the effect of non-Darcy seepage on productivity is much greater than that of stress sensitivity in the reservoir. Under the premise of not producing sand and not affecting energy supplement, the production wells could be exploited by enlarging production differential pressure as much as possible to obtain the higher productivity. The higher seepage capacity, oil-displacement efficiency and productivity could be obtained by timely and effective energy supplement in low permeability reservoirs. It is suggested to adopt the mode of advance or synchronous water injection to maintain pressure development in fault-block reservoirs with low permeability. The established productivity prediction equation can well characterize the productivity change rules of the low-permeability test well. Meanwhile, the variations of productivity are predicted under different effective permeability and maintenance levels of formation pressure. Based on various effective permeability setting, test duration of exploration wells and prediction of production index in the reservoir, it suggests that the stable productivity is 71.4% of the test productivity, under the condition of maintaining pressure development in target reservoir.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS03 / 87

A wave-mediated effective diffusion model for gas production from a semi-sealed system

Authors: Yan Jin[1]; Shiming Wei[1]; Kangping Chen[2]

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Massive hydraulic fracturing has made economical production from well-compacted deep geological formations such as shale possible. Despite the commercial success, the physical mechanisms

for the significantly enhanced production rate versus the conventional models remains unresolved. The mass flow from the matrix blocks to their adjacent fractures are the sources fed to the fracture network as well as the bottleneck of this semi-sealed production system. Earlier studies attribute the enhanced flow rate from the matrix blocks to the fractures to slip flow and Knudsen diffusion within the matrix blocks. Patzek [1], on the other hand, has argued that Knudsen-like scaling model is inappropriate for describing gas flow in tight formations such as shale. He demonstrated that the effect of slip on gas flow in tight formations is very weak. Both slip flow and Knudsen diffusion are only suitable for describing rarefied gas flows, but not for shale gas, which is under very high pressure in deep formations. Similar arguments on the unsuitability of the slip model for shale gas were also provided by Chen & Shen [2]. Gas flow from the matrix block to the adjacent fractures is a problem of production from a semi-sealed system. For such a system, our previous works based on the pore-scale compressible Navier-Stokes equations have shown that the motion of a viscous compressible gas is governed by a damped wave equation, and it exhibits a slip-like mass flow rate with a no-slip velocity profile [2-6]. Here we numerically and experimentally investigate how the rarefaction wave initiated at the start-up of gas flow affect the gas production from a semi-sealed dense porous plug. When a wave tries to penetrate a dense random porous medium, it loses its coherence and degenerates to a diffusion front beyond the so-called penetration length, resulting from repeated random reflections of the wave from the solid surfaces in a dense porous medium. Effective diffusion models have been long used by the physics community to describe such gas transport [7-14]. In our work, rarefaction wave induced gas transport at the pore-scale is first numerically simulated in randomly distributed porous media. By matching the computed macroscale mass flow rate with the one computed using a macroscale diffusion equation, the effective diffusion coefficient and its structure can be identified. With a large number of such computations, a machine learning model is established to extract the dependence of the effective diffusion coefficient on the mean radius and the variance of the solid grain, the porosity of the porous medium and the ratio of the outlet to the mean radius of the solid grain. A laboratory scale gas production experiment is then carried out to validate the effective diffusion model. Comparison between the model and the experiments shows that the wave-mediated effective diffusion model provides significantly better predictions for the gas production rate than that based on the Darcy's law. The newly proposed wave-mediated effective diffusion model is therefore promising for applications to gas production from semi-sealed systems with fractured networks.

Participation:

In-Person

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Simulation Research on the Profile Control Mechanism of Foam Fluid in Fractured Reservoirs

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Fractured reservoirs are generally dual medium reservoirs, which have two types of reservoir spaces with completely different porosity and permeability. After the oil and gas resources in the fractures are displaced out rapidly, the production declines quickly. For the fracture network with strong heterogeneity, effective profile control is required to improve the sweep efficiency in the fracture system to improve the reservoir heterogeneity and improve the water injection development efficiency. Foam can effectively solve these problems, but there are still some blind spots in the mechanism, further research on the plugging and profile control mechanism of foam fluid in fractured reservoirs is needed. In view of this, the level set method was used to carry out a simulation study on the control mechanism of foam fluid in fractured reservoirs, including the plugging effect of different fracture forms, the profile control effect of natural fractures with different fracture openings, and the profile control effect of micro fractures with different permeability. First, the flow field, pressure field, inlet pressure and foam texture of natural fractures, artificial fractures and high permeability microfractures are compared. This part mainly analyzes the plugging performance of foam fluid in fractured reservoirs. Secondly, for natural fractures with different opening ratios and matrix core combinations, the comparative analysis of natural fractures with different opening ratios is carried out, focusing on the changes in velocity, pressure and diversion rate. This part mainly determines the applicability of foam fluid for profile control of fracture size. Thirdly, the velocity field, pressure field and foam texture of the three core structures of matrix, homogeneous and high permeability strip are compared and analyzed, and the changes of velocity and pressure with time are studied. This part mainly explores the profile control mechanism of foam fluid in complex fracture zones. The research results show that artificial fractures and high permeability micro fractures are denser than natural fractures, the Jamin effect produced by foam is stronger and the secondary foaming ability is better, more foam accumulates in pores, and the plugging ability of foam to natural fractures is far less than that to artificial fractures and high permeability micro fractures; With the increase of fracture opening ratio, it is more and more difficult for foam to block large fractures. foam has good profile control effect when the opening ratio is 4:1, 2:1, and even the diversion rate turns over. However, at 10:1, the profile control and diversion effect are bad, and it cannot play an effective role in profile control; The foam first blocks the high permeability area, so that more follow-up fluid enters the low permeability area. This study provides theoretical support for the effective application of foam fluid in fractured reservoirs.

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MS08 / **89**

Adaptive models for nonlinear flows in highly heterogeneous porous media

Authors: Francesco Patacchini[1]; Alessio Fumagalli[2]

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Underground storage of gas (H2, CO2, etc.) and geothermal energy has become a major research area in the ongoing energy transition. In this context, it is important to model and simulate single- and multiphase flows in highly heterogeneous porous media, characterized by very irregularly distributed permeability profiles featuring fractures, channels and macropores.

Flows in these media might not follow Darcy's law; Forchheimer's quadratic law is more adequate in the high-Reynolds zones, and applying it globally in the domain is very accurate but costly numerically because of the nonlinearity introduced. Instead, keeping Forchheimer's law only where necessary should improve computing cost without losing much accuracy. The difficulty with coupling the two laws lies in determining which regions of the porous medium require Forchheimer's model and which ones can be treated linearly, a question with no clear answer yet.

Two adaptive models have been recently proposed to couple the two laws and answer the above question; given a fixed threshold on the flow velocity's magnitude, these models locally select the more appropriate law as they are being solved. At the end, each mesh cell is flagged as being in the Darcy or Forchheimer subdomain.

In the first model [1], the interface separating the two subdomains is tracked throughout a fixed-point algorithm. More precisely, the velocity is iteratively re-evaluated and, comparing the velocity' s magnitude to the fixed threshold, the cells are reflagged as being Darcy or Forchheimer cells. Also, a remeshing is performed: if the opposite edges of a cell have velocities with higher and lower magnitudes than the threshold, then the interface is moved at the center of the cell and a new mesh is generated such that the interface coincides with the edge of two newly created neighboring cells.

In the second model [2], the interface is not localized sharply. Instead, a regularized law is introduced resulting from a smooth average of Darcy's and Forchheimer's laws; this law gradually passes from Darcy's to Forchheimer's, and vice-versa, in so-called transition zones which surround the interface. A classical fixed-point algorithm is then directly run on the regularized law.

In this presentation, we will define these two models in detail, prove their well-posedness using tools from monotone operator theory and variational calculus, and illustrate their behavior via some numerical results obtained on simple, preliminary one- and two-dimensional test cases.

Participation:

In-Person

References:

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Poster / 90

Adaptive node adjustment for real-time subsurface flow modeling

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Real-time subsurface flow simulation is desirable for managing groundwater resources, geothermal exploitation, carbon dioxide geological sequestration, or underground hydrogen storage. Data assimilation methods are developed to achieve this goal. However, assimilation models usually use mesh-based numerical methods. Remeshing is frequently required whenever new data to be integrated into the model are not located at the existing computational nodes. This study aims to develop an adaptation algorithm to accommodate node layout to the exact positions of additional data. For flexibility, we chose a mesh-free numerical method. We combined it with a fast node generation technique called the advancing front method to adjust meshless node placement before assimilation by ensemble Kalman filter. A hypothetical flow problem was used to test the proposed approach. The results show that the adaptive node adjustment works effectively for the real-time updating model. The accuracy and precision of modeling states and parameters were improved when integrating additional data.

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Impact of wettability alteration on salt transport and mixing during low-salinity waterflooding

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Low-Salinity Waterflooding (LSWF) has been proven to be an efficient enhanced oil recovery (EOR) method which improves sweep efficiency by altering the reservoir rock wettability toward a more water-wet state. Wettability alteration is believed to be the main phenomenon behind the incremental oil production during LSWF. The impact of wettability and wettability alteration on salt transport has not been investigated so far, to the best of our knowledge. Since salt dispersion and mixing, which is believed to be one of the main challenges of LSWF, may be affected by wettability alteration, a proper understanding on the impact of wettability alteration on salt dispersion is necessary to have a proper design for this process.

In this study, a series of two-phase sandpack flooding tests was performed to investigate the impact of wettability alteration on salt transport during LSWF through recording breakthrough curves. In this regard, a 25cm long sandpack was first flooded with high-salinity water (100,000 ppm NaCl). Once a uniform salinity profile was obtained within the porous medium, crude oil was flooded into the sandpack to establish irreducible water saturation, which mimics the initial condition of the oil reservoirs. Next, in one test the core was aged at high temperature for 4 weeks and in one other test the core was not aged before waterflooding. Finally, low-salinity brine (2,000 ppm NaCl) was injected to both cores to displace the oil. Salinity of the effluent brine was recorded versus time to obtain breakthrough curves and investigate the impact of wettability alteration on salt transport.

Results of these two sandpack tests clearly show that the breakthrough curves are totally different in absence and presence of wettability alteration. For the test without aging and therefore in absence (or with a minimum degree) of wettability alteration, the breakthrough curve is somehow similar to the single-phase displacement of high salinity with low salinity and the effluent brine salinity reaches the injection salinity before injecting two pore volumes of the low-salinity brine. However, non-Fickian salt transport was observed due to the presence of the second phase (oil) and the results could not be just interpreted using simple advection-dispersion equation. For the system with aging and wettability alteration to a more water-wetting state, more than 3.5 pore volumes of low-salinity brine were necessary for the effluent brine salinity to reach the injection salinity. The contribution of wettability alteration during LSWF could be easily identified through the shape of the breakthrough curves. Wettability alteration makes the salinity profile curve much more asymmetric with a long-lasting tail, which is caused by the contribution of the released oil from new pores, and the released high-salinity brine from the smaller pores due to the altered wettability.

The results clearly show that although incremental oil recovery is obtained by LSWF due to wettability alteration, salt transport would be more dispersive. Thus, a larger low salinity slug size should be considered for a system with a greater change in the wettability state.

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MS10 / **92**

Nano-resolution X-CT 3D Imaging and Permeability Simulation of an Actual Shale Kaolinite

Author: Anderson Camargo Moreira[1]

Co-authors: Celso Peres Fernandes [1]; Rodrigo Surmas [2]; Iara Frangiotti Mantovani [1]; Lucas Debatin Vieira [3]; Hannes Claes [4]

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Pore and pore network characterization in clays and claystones is essential as they are of longtime and continuing importance in conventional hydrocarbon exploration, unconventional reservoirs and gas (e.g. CO2 and N2; Vernooij et al., 2020), and radioactive waste (Plúa et al., 2021) storage caprocks. Nonetheless, they also occur within the reservoir where they can act as local baffles (Benham et al., 2018) or exceptionally lie at the origin of secondary porosity generation like in the pre-salt formation offshore Brazil (Tosca and Wright, 2015). Porosity and permeability are key factors in assessing the hydrocarbon productivity of unconventional (as shales) reservoirs, which are complex due to their heterogeneous mineralogy and poorly connected nano- and micro-pore systems (Goral et al., 2020). Kaolinite is a kind of clay mineral from the kaolin group with an asymmetric structure similar to stacked layers of pseudo-hexagonal tiles, or platelets, with a few tens of nanometers in thickness (Brigatti et al., 2013; Varga, 2007, Johnston, 2010). Each of these platelets can be considered as an individual kaolinite crystal that can be stacked forming macrostructures (aggregates), as booklets and vermiform morphologies (Mansa et al., 2017). Numerical permeability simulations on these structures are quite rare due to the difficulty in properly imaging them. Due to their small dimensions, most of the registered images of kaolinites are achieved in 2D space with the SEM (scanning electron microscopy) technique (Ivanić et al., 2015; Mansa et al., 2017; Alcázar-Vara and Cortés-Monroy, 2018). This makes kaolinite (and clays in general) permeability estimation challenging since numerical simulations are performed with 3D images of the porous system, whether they are pore networks or voxel-based digital structures. Even though 3D models of shales reconstructed based on 2D image information can be performed (Chen et al., 2015), running simulations on an actual 3D image of the porous media represent a direct process, bypassing the modeling reconstruction. The relatively new focused ion beam (FIB) technology improves the SEM technique making it capable to provide 3D images in high resolution of samples such as clays (Zhu et al., 2021). However, an alternative to FIB-SEM and 3D modeling is high-resolution X-ray nanotomography (nanoCT). NanoCT performs image acquisition in the area of submicron X-ray tomography (Withers, 2007). Since X-ray microtomography (micrometer scale version of tomography) is often employed to analyze the 3D pore network structures of materials, nanoCT is a promising technique that aims to improve this analysis, enabling one to reach the nanometer scale. Besides improving qualitative insight into kaolinites by providing an actual 3D image of it on the nanoscale, this work also aimed to estimate its absolute permeability. A 117 m diameter cylindrical sample containing the kaolinite mineral was drilled from a shale sample with a laser ablation system and an Xradia/Zeiss nanoCT scanner UltraXRM-L200 was employed to generate images with 64nm/voxel spatial resolution. The lattice Boltzmann method was used to simulate permeability that was found to be 0.09 mD.

Participation:

In-Person

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Energy Transition Focused Abstracts:

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Geometric confinement stabilizes fluid invasion during imbibition in microfluidic porous media

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We establish a comprehensive description of the invading patterns formed when a wetting liquid displaces a non-wetting fluid in various porous mediums with geometric confinement variation. Building on model microfluidic experiments, we evidence imbibition scenarios yielding different imbibition stability and macroscopic morphologies controlled by geometric confinements and the capillary number. We report a phenomenon whereby no or weak depth variation of microfluidic porous media but with the strong geometric confinement suppresses flow instability during immiscible imbibition, that seemingly ignored or contradicts conventional expectations. Theoretical analytical models and pore-scale numerical simulations were combined for characteristics of imbibition front and final displacement result as a function of geometric confinements. We get a complete dynamic view of the imbibition process over a full range of regimes from the unstable patterns dominated by the snap-off or by-pass phenomenon to the stable state dominated by the cooperative pore filling. The study provides new insights into the role of geometric confinements in suppressing unwanted invasion instabilities in porous media. The finding provides design or prediction principles for engineered porous media, such as rock, exchange columns, fabric, membranes, and microfluidic devices concerning their desired immiscible imbibition behavior.

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MS01 / **94**

Energy Storage in Unconventional Formations

Authors: Hanin Samara[1]; Tatjana von Ostrowski[2]; Philip Jaeger[3]

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Objective:
The success of large-scale geological storage of gases requires proper understanding of the interfacial behavior among the participating phase. In this work a systematic study on the impact of pressure and brine salinity on the interfacial tension (IFT) of binary H2-brine systems as well as wettability within ternary systems comprising H2-brine-shale are investigated. Furthermore, the shale adsorption capacity of H2 is measured at elevated pressures up to 30 MPa. The conversion of the organic matter at elevated temperatures and elevated pressures under H2 atmosphere has also been examined to understand the role of hydrogenation in upgrading shale oil products.
Methods:

A high-pressure high-temperature view cell with a Pmax of 69 MPa and a Tmax of 200 ℃ (Eurotechnica GmbH,Germany) was employed to measure the IFT using the pendant drop method. The view cell was also employed to measure the wettability using the sessile drop method. A magnetic suspension balance (MSB) with Pmax of 40 MPa, Tmax of 150 ℃ (Rubotherm GmbH, Germany) was used to measure the adsorption of H2 on shale based on the gravimetric method. Thermal gravimetric analysis (TGA) was conducted using an MSB with Pmax of 15 MPa and 400 ℃ (IsoSORP, Waters TA instruments, Germany). The products of the TGA were analyzed using Nuclear Magnetic resonance (NMR) (Avance III 600 MHz-Bruker, Czech Republic) and Gas Chromatography (GC) (Varian 320-Agilent, United States).

Results, Conclusions:

The reduction in IFT upon increasing the pressure was insignificant. Further on, wetting tests suggest that the system is water wet under all experimental conditions. Both these findings guarantee the structural storage integrity of the shale. It is also found that adsorption plays a role in H2 storage within the shales. The NMR and GC analyses reveal that aliphatic compounds are excessively present in comparison to aromatics and olefinic compounds. In an H2 environment, it was observed that aromatic substitution by aliphatic hydrocarbons took place.

Novelty:

This work presents information on H2 wettability and H2 adsorption capacity of shale at conditions relevant to gas storage which are severely lacking in the literature. Furthermore, and up to the best of the author's knowledge, the conversion of organic matter at H2 pressures relevant to gas-storage is introduced for the first time.

Participation:

In-Person

References:

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MS06-B / 95

A molecular simulation study for interfacial tensions, solubilities, and transport properties of the H2/H2O/NaCl system relevant for Underground Hydrogen Storage

Author: Willemijn van Rooijen[1]

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Due to the intermittent nature of renewable energy resources like wind and solar, development of large-scale (TWh) energy storage systems is essential. A feasible solution for this can be offered by Underground Hydrogen Storage (UHS) in porous media. To ensure the safety of UHS, as well as to optimize injection and withdrawal cycles, a good understanding of hydrogen (H2)/brine interfacial, thermodynamic, and transport properties is needed [1]. More specifically, the diffusivities and solubilities of H2 in brine, and the interfacial tensions of H2 gas in contact with brine are crucial properties for reservoir simulation.

Traditionally, these thermophysical properties are measured experimentally. Based on the available experimental data, it is evident that only a limited range of the required interfacial tensions, solubilities, and self-diffusivities of the H2/H2O/NaCl system has been measured, while in some cases, there are significant discrepancies between the data reported from different sources. The reason for the scarcity of and deviation in the data may be that experimental measurements are rather challenging and expensive to perform, especially at high pressures and temperatures. To this end, molecular simulation is a widely used complementary approach for obtaining thermophysical data [2,3], especially at conditions which are challenging for experimental measurements.

In this work [4], force field-based Molecular Dynamics (MD) and Continuous Fractional Component Monte Carlo (CFCMC) simulations are carried out in this work to cover this gap. Extensive new data sets are provided for (a) Interfacial tensions of H2 gas in contact with aqueous NaCl solutions for temperatures of 298 - 523 K, pressures of 1 - 600 bar, and molalities of 0 - 6 mol NaCl/kg H2O computed using MD, (b) self-diffusivities of infinitely diluted H2 in aqueous NaCl solutions for temperatures of 298 - 723 K, pressures of 1 - 1000 bar, and molalities of 0 - 6 mol NaCl/kg H2O computed using MD, and (c) solubilities of H2 in aqueous NaCl solutions for temperatures of 298 - 363 K, pressures of 1 - 1000 bar, and molalities of 0 - 6 mol NaCl/kg H2O computed using CFCMC simulations. The simulations for computing H2 self-diffusivities are also used to yield predictions for densities and viscosities of the NaCl solutions.

Our results are validated against the available experimental data, models, and simulations. Excellent agreement between the results and experimental data is found with deviations smaller than 10% for most of the data points. The investigated properties depend on pressure, temperature, and salt concentration, with the exception of interfacial tension where no significant dependence on pressure was found. The dependencies were analysed and were in agreement with expectations based on theory and available literature. Using this analysis, we were able to develop engineering equations for interfacial tension and self-diffusion capturing the effect of pressure, temperature, and solution molality. These equations can be used in reservoir simulators for calculating values at a specific combination of conditions in a fast and reliable way.

Participation:

In-Person

References:

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Poster / 96

A Fourier-transform approach for fringe pattern analysis for a Mach-Zehnder interferometry measurement on surface evaporation of saturated porous media

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The interaction of fluids with different types of porous media plays an important role not only on our daily lives, but also understanding natural and industrial processes. Detailed studies of evaporation processes in porous materials are required not only to increase the fundamental understanding but also to enhance performance in engineering terms. The efficient design, operation and optimization of such engineering applications rely on detailed and thorough understanding of the interaction in terms of exchange of mass, momentum and energy. Several different techniques have been implemented to study this behaviour experimentally. Most experimental investigations are conducted using weight measurements, where a completely saturated porous probe is placed on a balance. However, local values of the surface evaporation flux are difficult to determine using this measurement technique. For this reason, we want to use an existing measurement technique, which is the interferometry, to estimate these local evaporation rates at the interface of a porous medium. This measurement technique has already been used to investigate drying processes on porous media [1, 2], but also to determine concentration gradients on evaporating droplets [3] and the evaporation of binary water-ethanol mixtures [4].

In this work, the evaporation of different fluids in a fully saturated porous medium is examined with a Mach-Zehnder interferometer. The latter uses the phase shift between two collimated light beams that results from splitting the light from a single light source due to a change in density or refractive index. The evaporation of moisture from the porous surface causes a deflection of the interference fringes, which thus leads to a phase shift. From this phase shift $\Delta\phi$, the change of refractive index Δn is computed using $\Delta n = \frac{\Delta\phi\lambda}{2\pi t}$ where λ is the wavelength of the light source, and t the depth of the measurement region. To extract the two-dimensional phase shift from the interferogram, the Fourier transform based approach by [6] is used. However, one of the problems of the approach used is that the phase-retrieval technique give the detected phase wrapped into the interval $[-\pi, \pi]$. This is due to the non-linear wrapping function involved in the phase-estimation process. Unwrapping is the process by which these discontinuities are resolved and the result is transformed into the desired continuous phase $\phi_{con}(x, y) = \phi(x, y) + 2\Pi k(x, y)$ where $k(x, y)$ is an array of integers. The unwrapping problem has been an important research topic for over decades [5]. For phase maps composed from consistent phase maps fringe data, there are many different algorithms, but there is none used for our type of problem. The questions that needs to be addressed to resolve the unwrapping problem is: under what circumstances can this lost information be recovered? The main objective of this work are these phase discontinuities and how they can be solved to reproduce the local evaporation rates at the surface of the porous models as accurately as possible.

Participation:

In-Person

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MS18 / **97**

Foam for Soil Remediation: Similarities and Differences with Foam for Hydrocarbon Recovery

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Foam has been studied and applied for enhanced oil recovery (EOR) for many decades. There is a large body of research on this topic (Kovscek and Radke, 1994; Rossen, 1996), from pore-level mechanisms of creation and destruction of bubbles and foam mobility to modelling foam processes on the laboratory and field scale. Foam is also increasingly receiving attention as a means of improving soil remediation (Bertin et al., 2017). This raises the question: what findings and modeling approaches that apply to foam for EOR apply to soil remediation, and which require major modification?
In EOR applications in the relatively deep subsurface, foam stability is controlled by capillary pressure. Bubbles are as large as pores, because of inter-bubble diffusion. As a result, foam exists in two flow regimes depending on flowing gas fraction (Alvarez et al., 2001). This is key to modelling foam for EOR.
In soil remediation, as in EOR, foam's primary purpose is to redirect the flow in the formation. In soil remediation, permeability is much greater, which means capillary pressure is less than in EOR. Foam bubbles are not trapped as easily as in EOR foam. Experiments show bubbles smaller than pores, and wet conditions in aquifers, make the effect of diffusion uncertain. As a result, whether the two flow regimes found for EOR foam apply to soil remediation is moot. The goal of EOR is to make a measurable increase in oil recovery; in soil remediation 100% recovery of toxic waste (NAPL) is the goal. Moreover, the remediation fluids must be recovered, not left in the formation. Foam for soil remediation is usually pregenerated before injection, but injection pressure is severely limited. As a result, aquifer flow and gravity play a much larger role in soil remediation than EOR.

Many aspects of foam apply to both applications. Gas mobility is greatly reduced in both cases, and gas trapping is significant in both. Capillary forces are critical at the pore scale, though they are likely to be less dominant at the higher permeabilities in soil remediation. The basic mechanisms of bubble creation are the same. Foam generation in gas flow across layer boundaries was found to be critical to the success of foam in one application to aquifer remediation (Hirasaki et al., 1997). The presentation will discuss how the physico-chemical processes described in EOR apply to environmental application, and if new phenomenon need to be considered specifically for soil remediation.

Participation:

In-Person

References:

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99

A Novel CO2 Geological Sequestration Technology: Geothermal Assisted CO2 Catalytic Reduction

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CO2 sequestration into geological formation was given great expectations in alleviating the aggravating greenhouse effect. However, the current CO2 geological sequestration technologies confronted many challenges in engineering, including the low sequestration efficiency, high leakage risk, and poor economic feasibility. Given this, a brand new CO2 geological sequestration technology, i.e., the geothermal assisted CO2 catalytic reduction (GT-CO2CR) was proposed and its feasibility, effect, and mechanism were investigated.
First, a large-scale CO2 sequestration apparatus which used the outcrop core (150cm×50cm×50cm)

and equipped with GT-CO2CR accessories was designed and constructed. Then, the CO2 sequestration experiments were performed using the water vapor with different temperatures to investigate the GT-CO2CR effects on CO2 sequestration. Accompanying, the core/liquid-nuclear magnetic resonance spectroscopy (NMR) were conducted to analyze the properties changes of core sample and injection brine for unraveling the GT-CO2CR mechanisms.
CO2 sequestration experiments indicated that GT-CO2CR remarkably enhances CO2 sequestration into geological formation and the temperature is critical. As temperature increases from 100℃ to 350℃, CO2 sequestration efficiency increases from 75.8% to the maximum of 92.2% at 250℃ and then decreases to 87.6%. Corresponding, their final pore pressures are 0.55, 0.31, and 0.43Mpa, respectively. Obviously, 250℃ is the optimal temperature. Core/liquid-NMR revealed that GT-CO2CR alters the properties of core sample and injection brine. Liquid-NMR indicated that CO2 is catalyzed into formate and the rate is as high as 45.2μmol/min at 250℃. Core-NMR illustrated that GT-CO2CR enlarges the pore-throat volume and the intensity enhances as the temperature increases. Herein, the main pore-throat radius within 100, 250, and 350℃ cases are 0.028, 0.041, and 0.048μm, respectively. Conclusively, inspired by the high temperature and catalysts, CO2 conversion into formate and pore-throat enlargement acted synergistically to enhance CO2 sequestration into geological formation.
This technology markedly elevated CO2 sequestration amount, stability, and safety, and provided an option for the future CO2 industrial sequestration.

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MS05 / 101

Life in a tight spot: How bacterial populations spread through porous media

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Bacterial spreading through motility and growth plays a central role in agriculture, biotechnology, the environment, and medicine. These processes are typically studied in the lab in liquid cultures or on flat surfaces; however, many bacterial habitats—e.g., soils, sediments, and biological gels/tissues—are more complex and crowded 3D porous media. In this talk, I will describe my group's work unravelling how confinement in a 3D porous medium changes how bacteria behave. We have developed the ability to (i) directly visualize bacteria from the scale of a single cell to that of an entire population, and (ii) 3D-print precisely structured multi-cellular communities, in crowded 3D porous media more akin to their natural habitats. Our experiments using this platform have revealed previously unknown ways in which crowding fundamentally alters how bacteria move and grow, both

at the single cell and population scales. Guided by these findings, we have developed theoretical models to more accurately predict the motion and growth of bacterial populations, and other forms of "active matter", in complex porous media. Taken together, these findings help to reveal new principles to predict and control the organization of bacteria, and active matter in general, in complex and crowded environments. They could also potentially help provide quantitative guidelines for the control of these dynamics in processes ranging from bioremediation and agriculture to drug delivery.

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MS16 / 103

Vapor and bound water transport in textiles and paper: observation by MRI and modelling

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Textiles and paper are ubiquitous in our daily lives. The comfort of clothing is essentially determined by the hygrothermal behavior of textiles, as fabric sorption clothing can play a significant role in the moisture transport and heat loss caused by sweating. For paper production, the extraction of the final bound water fraction consumes large amounts of energy, and the majority of the functional properties of paper are developed during this stage. To assist with the correct design and manufacture of textiles and paper, we must master the mechanisms of water transfers in them.
However, it is difficult to quantitatively investigate this phenomenon due to the lack of simple measurements of water distribution inside the material. One of the major complexities in the process investigation lies in the fact that for these hygroscopic materials, water molecules can be absorbed by the cellulose fibers from vapor in the surrounding air. Water transfers can occur as vapor diffusion in pore net-work and/or bound water diffusion in cellulosic fiber skeleton, with additional adsorption and desorption in such materials. Standard measurements rely on monitoring global mass variations of the sample under more or less controlled humidity boundary condition, but hardly distinguish the bound water diffusion from vapor diffusion.
Here, we have developed an original experimental technique based on Magnetic Resonance Imaging (MRI) and Macroscopic measurement to simultaneously monitor the water transfers in pure cellulose samples with various porosities. Firstly, with the help of Nuclear Magnetic Resonance (NMR), we have measured the bound water diffusion by drying a stack of cellulose fibers whose pore network was filled with olive oil, which blocks vapor diffusion. Surprisingly, it appears that there is in general a continuity of bound water diffusion through the cellulosic solid skeleton, and we can directly measure the diffusion coefficient of bound water. In a second step, we have implemented

specific tests under fully controlled boundary conditions (in terms of relative humidity) to estimate the vapor diffusion coefficient. The mass transport is deduced from the constant mass flux including vapor and bound water transfers through the sample once the steady state is reached. By subtracting the bound water diffusion flux from the global diffusion flux, we obtain the vapor diffusion flux and the corresponding diffusion coefficient.
Finally, the predictions of a simple diffusion model relying on the conservation of water-vapor mass to fully describe the transient water transfer process with both fluxes, and using these diffusion coefficients, are compared with saturation profiles at different times measured by MRI. The excellent agreement over a wide range of sample porosities validates our model and the obtained diffusion coefficients. We expect that this original experimental protocol opens a way for the characterization of fabric properties and that our results to be broadly useful for the textiles and paper manufacture.

Participation:

In-Person

References:

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104

Permeability Up-scaling of Digital Rocks via Physics-Informed Neural Networks

Author: Mohamed Elmorsy[1]

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Groundwater movement, oil extraction, and geological carbon dioxide sequestration are just a few examples of the many natural and industrial processes that depend on subsurface characteristics, such as the permeability of fluid flow through natural porous media. Over time, scientists and engineers have worked to find efficient ways to determine these characteristics. Recently, digital technologies like three-dimensional (3D) imaging of core samples have been developed to enable digital subsurface characterization, which will speed up and improve the process of subsurface characterization. Due to the tremendous computational cost, digital characterization of porous media using 3D numerical simulations is still restricted to digital samples much smaller than the Representative Elementary Volume (REV). Here, we present a new analytical solution to upscale the permeability of digital rocks made of anisotropic blocks. Additionally, we introduce a neural network framework that is tested and trained on a variety of rock types, including the Berea sandstone, Bentheimer sandstone, and Keton limestone, covering a wide range of permeabilities (i.e., 1000 to 5000 mD). The model accurately predicts the permeabilities of samples with a size of 600 x 600 x 600 voxels based on the permeabilities of subsamples with a size of 150 x 150 x 150 voxels.

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Poster / 106

Characterization shale's pore structure of shale: Multi-experimental imaging technique with machine learning

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Shale oil and gas is becoming increasingly crucial for unconventional oil and gas exploration and development worldwide. The pore structure determines the transport properties in shale oil and gas reservoirs, which affects the assessment and development of shale oil and gas potential. Shale oil and gas reservoirs develop multi-scale and multi-type pore structures ranging from nanometers to millimeters, divided into micro-fracture, organic, and inorganic pore space. To wholly and precisely comprehend the pore structure of shale from the nano- to the micro-scale, this paper proposed a multi-experimental imaging technique, including X-ray computed tomography (XCT), large field of view scanning electron microscopy (SEM—Maps), and focused ion beam scanning electron microscopy (FIB—SEM), to establish a multi-experimental imaging workflow for shale. The combined imaging workflow was used to obtain two-dimensional (2D) and three-dimensional (3D) multi-resolution images of shale. Data fusion to combine different resolution XCT, SEM—Maps, and FIB—SEM images with machine learning methods to characterize the multi-scale pore structure of shale oil and gas reservoirs. The multi-dimensional and multi-resolution shale images were performed at single-scale and multi-scale simultaneously. The results showed that shale pores mainly consist of micro-fractures, inorganic pores, organic matter, and organic pores. All of them exhibit multi-scale characteristics. Organic matter shows strip and bulk distribution, and organic pores are not found in a large amount of organic matter. The multi-scale pore structure of shale was described quantitatively. The pore radius less than 10 nm accounts for 16%, 10-20 nm accounts for 18%, 20-50 nm accounts for 20%, 50-100 nm accounts for 23%, 100-500 nm accounts for 11%, and 500 nm-20 μm accounts for 6%, 20-50 μm accounts for 5%, 50-100 μm accounts for 1%. Inorganic matter pores are of various types, among which extensively produced dissolving pores. Finally, the connectivity of organic pores is poorer than inorganic pores. The connectivity between organic and inorganic pores plays a crucial role in oil and gas storage, while micro-fractures dominate the fluid flow channels. Organic pores dominate the Pore radius of shale <50nm, the pore radius of shale between 50~500nm are organic pores and inorganic pores, and the pore radius of shale >500nm is mainly contributed by micro-fractures. The method proposed in this paper can effectively obtain the multi-scale pore structure of shale.

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MS13 / 109

Fluid transfers in nanopores through dynamic NMR relaxometry

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NMR relaxation time measurement is a well-known, non-destructive method to probe all states of protonic liquid such as water, in porous media, at different pore scales. In contrast with MRI which can get local information but is blind with respect to most liquid in nanomaterials, standard NMR relaxation measurements can provide information on the liquid content over six decades of relaxation times typically corresponding to pore scales from the millimeter to the nanometer. Here, we propose a simple though powerful technique which provides various direct, quantitative information on the liquid distribution inside nanoporous porous structures and its variations over time due to fluid transports and/or phase changes. It relies on the analysis of the details of the NMR (nuclear magnetic resonance) relaxation of the proton spins of the liquid molecules and its evolution during some process such as imbibition, drying, phase change, etc, of the sample. We present a few applications of this technique to nanoporous materials such as a silica glass [2], cellulose fibers [3], or nanoporous glass beads [1]. We show that this approach allows to observe and quantify a variety of possible dynamic phenomena such as: a progressive homogeneous or inhomogeneous emptying of pores, and isotropic or differential shrinkage of the pores, the possible existence of liquid films along the pore walls, transfers between bound and free water.

Participation:

In-Person

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MS15 / **110**

Simulating water flow and solute transport at unsaturated soils with unknown initial conditions using physics-informed neural networks trained with time-lapse geoelectrical measurements

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Accurate modeling of water flow and solute transport in unsaturated soils are of significant importance for precision agriculture and environmental protection. However, traditional modeling approaches are considerably challenging since they require well-defined boundaries and initial conditions. Harnessing machine-learning techniques, specifically deep neural networks (DNNs), to detect water flow and solute transport in porous media have recently gained considerable attention [1]. In traditional DNNs, an artificial neural network with several hidden layers is trained solely using data to approximate parameter and state estimation, e.g., the spatiotemporal distribution of water content and pore-water salinity. However, data is extremely limited and sparsely available in subsurface applications. Physics-informed neural networks (PINNs) have recently been developed to learn and solve forward and inverse problems constrained to a set of partial differential equations (PDEs). Unlike traditional DNNs, PINNs are confined to physics and do not require" big" data for training [2]. However, hydrological applications of PINNs only considered an in-silico environment with spatial measurements of hydraulic head, water content and/or solute concentrations well distributed in the subsurface [3]. Such measurements are hard to obtain in real-world applications since they require drilling to extract soil samples or installing in-situ measurement devices at depth which also violets the soil's natural structure. As opposed to conventional subsurface characterization and monitoring techniques, non-invasive geoelectrical methods can provide continuous, extensive, and non-invasive information of the subsurface [4]. Nevertheless, the sensitivity of the measured electrical signal to various soil parameters, mainly water content and pore-water salinity, as well as inversion errors, could result in biased hydrological interpretations.

This work adopted the PINNs framework to simulate two-dimensional water flow and solute transport during a drip irrigation event and the following redistribution stage, using time-lapse geoelectrical measurements with unknown initial conditions. For that manner, a PINNs system containing two coupled feed-forward DNNs was constructed, describing the spatiotemporal distribution of both water content and pore-water salinity. The system was trained by minimizing the loss function, which incorporates physics-informed penalties, i.e., mismatch with the governing PDEs and boundary conditions, and measurement penalties, i.e., mismatch with the geoelectrical data. Two-dimensional flow and transport numerical simulations conducted with the Hydrus 2D/3D software [5] were used as benchmarks to examine the suitability of the described approach.

Results have shown that the trained PINNs system was able to reproduce the spatiotemporal distribution of both water content and pore-water salinity during both stages, i.e., irrigation and redistribution, with high accuracy, using five time-lapse geoelectrical measurements conducted with 59 electrodes placed at the surface. The trained PINNs system also reconstructed the initial conditions of both state parameters for both stages. It was also able to separate the "measured" electrical signal into its two components, i.e., water content and pore-water salinity. In addition, the subsurface geoelectrical tomograms were significantly improved compared to those obtained from a classical inversion of the raw geoelectrical data.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS15 / 111

Optimization of the CO2 injection location in heterogeneous siliciclastic reservoirs using graph theory

Author: Achyut Mishra[1]

Co-author: Ralf Haese [1]

[1] *The University of Melbourne*

Corresponding Authors: ralf.haese@unimelb.edu.au, achyut.mishra@unimelb.edu.au

Siliciclastic CO2 storage reservoirs often comprise lithological heterogeneity across different spatial scales. Consequently, the reservoirs could include high permeability pathways resulting in an unexpected migration of fluid. On the contrary, the presence of certain rock types which act as flow barrier, especially near the injection source, could block the flow of CO2 leading to reservoir pressure build-up. The latter is not desirable as it limits the CO2 injection rate. Identifying suitable injection locations away from flow barriers could require numerous high-fidelity numerical simulations due to the uncertainty resulting from the distribution of low-permeability rock types. This study presents a new computationally efficient approach for screening favourable locations for CO2 injection in heterogeneous reservoirs to minimise pressure build-up. The approach utilizes graph theory to identify the path of the least resistance to CO2 flow between the injection source and the top of the reservoir. Graph network models were synthetically created for 50 reservoirs to capture

the variability in rock properties and their distribution. The paths of least resistance were determined for these reservoirs and their characteristics were found to correlate with injectivity indices determined from numerical simulations on the same models. The correlation was further used to derive a classification criterion for predicting a grid-cell scale injectivity index in heterogeneous siliciclastic reservoirs. Testing showed that the approach could accurately predict the spatial variability of injectivity index with a computational boost of up to 10,000 times compared to the conventional numerical simulation-based approach.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS05 / **112**

Study of Biofilm Structure using Advanced Imaging Techniques and Extraction of Pore Network from Simulated Biofilms

Author: Emad Aamer[1]

Co-authors: Katja Bettenbrock [2]; Robert Dürr [3]; Lars Beyer [1]; Achim Kienle [4]; Nicole Vorhauer-Huget [1]

[1] *Otto-von-Guericke University, Magdeburg/Germany*

[2] *Max-Planck-Institute for Dynamics of Complex Technical Systems, Magdeburg/Germany*

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Corresponding Authors: emad.aamer@ovgu.de, robert.duerr@h2.de, lars.beyer@ovgu.de, achim.kienle@ovgu.de, nicole.vorhauer-huget@ovgu.de, katja@mpi-magdeburg.mpg.de

Pore network models (PNMs) are reduced discrete mathematical models that are widely applied to study mass and heat transfer in porous media . Considering biofilms as a kind of a porous medium, with the inter-cellular space forming the pores, PNMs appear very suitable to study the transport of substrates and products through biofilms. In electrochemically active biofilms, additionally the transport of mediators or electrons can be investigated. Biofilm morphology is quantified by using advanced imaging techniques like X-ray tomography, Confocal laser scanning microscopy (CLSM), and Scanning electron microscopy (SEM). The morphological parameters are then used to generate in-silico biofilms using averaging data on layer thickness, cell number, porosity and cell orientation. Different growth mechanisms result in different cell arrangements within the biofilm layers. The simulated biofilms are used to extract the pore networks, which form the base for the simulation of transport properties. This is shown in Fig. 1, where the PNM (on the right in blue) is reconstructed from the simulated biofilm. The mathematical method has the advantage that a wide range of biofilm structures can be studied in short time without high experimental efforts. The results are useful to understand the transport processes inside biofilms under different conditions and could be employed

to predict optimal process conditions for highly efficient processes, i.e. based on optimized single or multispecies biofilm developments.

Figure 1: a) Simulation of several layers of biofilm and (b) extraction of the pore network.

Participation:

In-Person

References:

Q. Xiong, T. G. Baychev, and A. P. Jivkov, Review of pore network modelling of porous media: Experimental characterisations, network constructions and applications to reactive transport, J. Contam. Hydrol., 192, 101–117, 2016.

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113

Pore-scale study of solid phase emergence and mass transfer processes during DNAPL remediation

Authors: Zejun Wang[1]; Zhibing Yang[1]; Ran Hu[1]; Yi-Feng Chen[1]

[1] *Wuhan University*

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Fundamental understanding of phase emergence and interphase mass transfer processes is of great importance for improving the treatment efficiency of in-situ contaminant remediation. We perform microfluidic experiments to study the pore-scale dynamics and phase evolution during DNAPL remediation by chemical oxidation and surfactant flushing. During chemical oxidation, we visualize the remediation evolution under the influence of solid phase emergence and explore the roles of injection rate, oxidant concentration and stabilization supplement. Combining image processing, pressure analysis and stoichiometry calculations, we provide comprehensive descriptions of the oxidant concentration-dependent growth patterns of the solid phase and their impact on the chemical reactions and remediation efficiency. During surfactant flushing, we characterize the droplet breakup behavior and the subsequent micro-movement of daughter blobs. Based on measurements and calculation of DNAPL saturation, interfacial area and mass transfer rate coefficient, we observe the inhibition of mass transfer rate coefficient when surfactant content is above critical micelle concentration. We finally propose a new mass transfer correlation model, which explicitly considers the surfactant inhibition effect and distinguishes itself from the previous mass transfer correlations.

Participation:

Online

References:

Wang, Z., Yang, Z., Fagerlund, F., Zhong, H., Hu, R., Niemi, A., Illangasekare, T., Chen, Y., 2022. Pore-Scale Mechanisms of Solid Phase Emergence During DNAPL Remediation by Chemical Oxidation. Environ. Sci. Technol. 56 (16), 11343–11353. https://doi.org/10.1021/acs.est.2c01311

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MS01 / **114**

Water vapor transport in porous salt hydrate particles in view of energy storage

Author: Joey Aarts[1]

Co-authors: Stan de Jong [2]; Pim Donkers [3]; Hartmut Fischer [4]; Martina Cotti [2]; Olaf Adan [4]; Henk Huinink [1]

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[2] *TU/e*

[3] *Cellcius*

[4] *TNO*

Corresponding Authors: s.j.d.jong@student.tue.nl, pim.donkers@cellcius.com, j.aarts@tue.nl, m.l.cotti@tue.nl, hartmut.fischer@tno.nl, olaf.adan@tno.nl, h.p.huinink@tue.nl

Due to a mismatch in energy production and energy demand a loss free method of storing energy is required. One class of materials suitable for this are salt hydrates. Salt hydrates release energy in the form of heat when subjected to water vapor by incorporating this water inside the crystal lattice (hydration/discharging). When subjecting the hydrated material to heat water is removed from the crystal lattice (dehydration/charging).

For effective use of salt hydrates inside a reactor bed mm-sized porous particles are required instead of powder, due to a high pressure drop over a powder bed. Since the pore structure influences water vapor transport and hydration, understanding the precise transport processes is critical.

The internal pore structure can be affected by several factor such as manufacturing conditions, morphology changes during cyclic loading and (re-)crystallization during hydration and dehydration.

First, it will be shown that the hydration of salt hydrate particles is diffusion limited. The porosity is the main parameter for tuning the effective diffusion coefficients for water vapor transport and power output as described in Aarts et al. (2022).

Next, the influence of cyclic dehydration/hydration and geometrical changes on the changes in pore structure and water vapor transport will be elucidated.

Lastly, it will be discussed how this influences the power output and performance as energy storage material for a single particle as well as a complete reactor bed.

Participation:

In-Person

References:

J. Aarts et al., "Diffusion limited hydration kinetics of millimeter sized salt hydrate particles for thermochemical heat storage,"J. Energy Storage, vol. 47, no. November 2021, p. 103554, Mar. 2022, doi: 10.1016/j.est.2021.103554.

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115

Impact of the stiffness contrast on the rupture of injection-induced earthquakes

Authors: David Santillan Sanchez[1]; Juan Diego Valadés[2]; Juan Carlos Mosquera Feijoo[3]; Luis Cueto-Felgueroso[1]

[1] *Universidad Politecnica de Madrid*

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[3] *Universidad Politécnica de Madrid*

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Injection-induced seismicity has emerged as a central scientific and societal issue in the development of subsurface energy technologies such as enhanced geothermal energy extraction, unconventional hydrocarbon production, wastewater injection, geologic carbon sequestration, or underground gas storage. Although our knowledge of induced seismicity has increased thanks to field observations and computational models, some key aspects remain poorly understood. One of the outstanding questions is how the stiffness contrast in the host rock impacts the nucleation and rupture of injection-induced earthquakes.
Here, we study the effect of the stiffness contrast in the host rock on the rupture of injection-induced earthquakes. We develop a computational model to simulate the dynamic response of a fault immersed in a fluid-saturated medium. We find that the stiffness contrast drives the undrained response on the fault during the rupture. The increase in the stiffness contrast promotes higher maximum displacement steps and asymmetric ruptures. Seismic moment also increases with the stiffness contrast, but time to rupture decreases.
Acknowledgements
This research was supported by the Comunidad de Madrid through the call "Research Grants for Young Investigators"from "Universidad Politécnica de Madrid"under grant APOYO-JOVENES-21-6YB2DD-127-N6ZTY3, RSIEIH project, research program V PRICIT.

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Energy Transition Focused Abstracts:

116

Efficient Forecasting of Production Statistics Combining Single-phase and Multiphase Flow Models

Authors: Qinzhuo Liao[None]; Gensheng Li[None]; Gang Lei[None]

Corresponding Authors: lg1987cup@126.com, ligs_li@126.com, liaoqz@gmail.com

In order to capture detailed reservoir heterogeneity, geological models of subsurface formations are generally constructed at fine scales, which contains a large number of gridblocks. Uncertainty quantification, which usually requires running the reservoir model on multiple realizations/scenarios, can be computationally prohibitive on the fine-scale models, especially for multiphase flow models.

We present procedures in which only one fine-scale multiphase flow models are simulated, together with a relatively large number of single-phase flow models. In addition, the single-phase flow model can be further upscaled from fine-scale to coarse-scale to save computational effort. We aim to efficiently capture the production statistics (e.g., mean, standard deviation and cumulative distribution function) of multiple realizations. This approach uses a similar idea as in the multilevel Monte Carlo that samples are taken on different levels of accuracy, and the difference is that we use the low-fidelity (i.e., single-phase flow) model as a pre-selection process. The proposed method is rigorously tested on well-driven flow problems with different variances and spatial correlations of the permeability field. It can be used to calculate bottom-hole pressure, water injection rate, and oil and water production rate. It is able to forecast the well performance using just 1 realization, compared to more than 100 realizations using standard Monte Carlo methods.

Overall, the proposed method is shown to reproduce the ensemble statistics of fine-scale results, with a computational speedup of more than two order of magnitude. It also serves a potential tool for optimization considering parametric uncertainty and probability.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS20 / **117**

Impact of large periodic deformations on solute transport in soft porous media

Authors: Matilde Fiori[1]; Chris MacMinn[1]; Satyajit Pramanik[2]

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From soils to soft biological tissues, there are many examples of materials that can be modelled as highly deformable porous media, characterised by a strong coupling between mechanical stimulation and fluid flow due to complex rearrangements of the pore space. In both contexts –subsurface geomechanics and living-tissue biomechanics or tissue engineering –the effects of large periodic deformations on solute transport and mixing can be of great interest for predicting and/or controlling the motion of contaminants or nutrients. Here, we propose a 1D continuum model based on large-deformation poroelasticiy that links an applied periodic deformation to the resulting solute transport and mixing. Transport occurs through advection, molecular diffusion, and hydrodynamic dispersion, all of which are affected by the deformation in specific ways. We explore the effects of several dimensionless parameters on the problem, focusing on the ones regulating the applied periodic load. We find that the amplitude and period of deformation influence the mechanical response of the material, which can belong to either a linear slow-loading or a nonlinear fast-loading regime. These mechanical regimes directly characterise the resultant movements of solute.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-B / **118**

Experimental investigation of two-phase flow with a table-top optical scanner: the competition between viscous and gravitational effects under different boundary conditions

Authors: Joachim Falck Brodin[1]; Per Arne Rikvold[2]; Marcel Moura[2]; Renaud Toussaint[3]; Knut Jorgen Maloy[4]

[1] *PoreLab, Physics Dept., The University of Oslo*

[2] *PoreLab - University of Oslo*

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We present experimental results of the development of a hydrodynamic instability in a 3D flow setup in which one fluid phase invades a porous network saturated with another fluid phase. The invading phase is both more viscous and more dense than the defending phase and the developing invasion pattern is governed by the balance between viscous and gravitational forces. The full invading front is made visible by means of a newly developed table-top 3D scanner based on optical index matching and laser-induced fluorescence [1]. The force balance in the problem predicts a transition between a stabilized compact front (viscous dominated flows) and an unstable fingering regime (gravity dominated flows). We consider two inlet boundary conditions that lead to either the flow diverging from a point source or initialized as a flat front. For the latter condition, the invasion front is extracted and we measure its fractal dimension.

Participation:

In-Person

References:

[1] J. F. Brodin, P. A. Rikvold, M. Moura, R. Toussaint and K. J. Måløy, "Competing Gravitational and Viscous Effects in 3D Two-Phase Flow Investigated With a Table-Top Optical Scanner," Front. Phys. 10, 936915 (2022).

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Energy Transition Focused Abstracts:

119

Experimental Study of Liquid Cohesion Effect on Particle Clogging in Rock Fractures

Author: Renjun Zhang[1]

Co-authors: Zhibing Yang [1]; Russ Detwiler [2]; Dongqi Li [3]; Gang Ma [1]; Ran Hu [1]; Yi-Feng Chen [1]

[1] *Wuhan University*

[2] *University of California, Irvine*

[3] *School of water resources and hydropower engineering, wuhan university*

Corresponding Authors: csyfchen@whu.edu.cn, detwiler@uci.edu, rjzhang@whu.edu.cn, magang630@whu.edu.cn, zbyang@whu.edu.cn, lidongqi@whu.edu.cn, whuran@whu.edu.cn

Suspension migration and particle clogging processes in rock fractures are ubiquitous in nature and industrial activities. Understanding the mechanism behind these processes is of great importance for improving the efficiency of various engineering applications such as hydraulic fracturing and hole-drilling fluid leakage resistance. We perform visualized experiments to investigate the effect of liquid cohesion on particle clogging in rough fractures. Four patterns of particle clogging behaviors are found as we vary the flowrate and secondary liquid content. It is observed that by simply adding a small amount of immiscible liquid phase into the particle suspension, the clogging in fractures is significantly enhanced due to capillary cohesion induced particle agglomeration. To quantify the effect of capillary cohesion induced by the additional immiscible liquid, we propose a theoretical

model of agglomerate size as a function of ω and a criterion of particle agglomerate size for particle clogging. The findings in this work can have potential applications in a number of field applications, including oil/gas exploitation, drilling fluid leakage resistance, and rock grouting, etc., where suspension migration and clogging processes in fractured rocks are involved.

Participation:

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Energy Transition Focused Abstracts:

Poster / 120

Particle methods for the dynamics of porous biofilms with heterogeneous rheology and its interaction with human lung epithelium

Authors: Jean-Matthieu Etancelin[1]; Marlène Murris-Espin[2]; Philippe Poncet[1]

[1] *University Pau & Pays Adour, France*

[2] *CHU Toulouse-Larrey, France*

Corresponding Authors: murris.m@chu-toulouse.fr, philippe.poncet@univ-pau.fr, jean-matthieu.etancelin@univ-pau.fr

In this presentation we are interested in operational applications and new numerical approaches for modeling the heterogeneous mucus bio-film of human lungs for the monitoring of cystic fibrosis (CF) therapies. At an operational level, we aim at predicting whether a therapy has a significant impact of the mucociliary clearance or not, that is to say predicting the ability of the respiratory mucus to be functional, i.e. to move together with the motion of the surrounding cells. By opposition, a non-functional mucus will not move sufficiently to clear the lung wall from allergens, toxic agents, viruses, bacteria and their residual products (DNA filaments and altered mucoid elements).

In this biological configuration, the mucus is itself a porous media made of Newtonian periciliary fluid (PCL) and highly concentrated mucins produced by the goblet cells, whose motion in the mucus will allow a mixture between the mucins and the PCL leading by reaction to a polymerized mucus with a particular rheology. Among the rheological features such as visco-elasticity, visco-plasticity, yield stress and shear-thinning, we focus on this last one which has been shown to be the dominant feature leading to non-functional mucus [3]. Moreover, the PCL is produced by the respiratory epithelium covering the lung membrane, another porous media that allows the transcytosis mechanism producing the PCL. Indeed, the PCL is not present or not working properly when the cystic fibrosis transmembrane conductance regulator protein CFTR presents a mutation responsible of CF.

The numerical simulation of such configurations has two main objectives. On the one hand, one can predict whether a mucus is functional or not, with respect to the rheological features that are measured from samples [4]. On the other hand, the numerical simulation allows to adjust the parameters of an upscaled model, including the mucus permeability and the tortuosity index that relates

the effective diffusion and the molecular diffusion of chemical species by means of a power of the porosity.

The mucus mixing is modeled by $-div(2\mu(c,D)\,D(u)) = f - \nabla p$, the non-Newtonian stationary Stokes equation, where f is the driving force induced by the epithelial cell, μ is mucus viscosity, $D = (\nabla u + \nabla u^T)/2$ is the shear-rate of the velocity u, p is the pressure, and the incompressibility is satisfied by $div(u) = 0$. The mucin concentration $c(x,t)$ follows
$\frac{\partial c}{\partial t} + div(uc) - div(\sigma\nabla(c)) = 0$
and the shear-thinning rheology is driven by the relation
$\mu(c,D) = \mu_\infty + (\mu_0(c) - \mu_\infty)\left(1 + 2\beta(c)^2|D|^2\right)^{\frac{q(c)-2}{2}}$
which makes all these equations strongly coupled. We will show that the solutions of this system can be expressed by a Lagrangian formulation [1,2], called particle method, that the numerical result are compatible with clinical resume of the patients whose sputum rheology has been characterized [4], and that the upscaled tortuosity index can be carried out.

This work has been funded by French National Agency of Research, project MucoReaDy ANR-20-CE45-0022-01, and by Carnot Institute ISIFoR project MicroMineral P450902ISI.

Participation:

In-Person

References:

[1] J.M. Etancelin, P. Moonen, P. Poncet, Improvement of remeshed Lagrangian methods for the simulation of dissolution processes at pore-scale, Advances in Water Resources, 146:103780, 2020. DOI: 10.1016/j.advwatres.2020.103780

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Energy Transition Focused Abstracts:

MS07 / 121

Recent Contributions to the Study of Immiscible Viscous Fingering

Authors: Kenneth Sorbie[1]; Alan Beteta[None]; Arne Skauge[None]

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Corresponding Authors: a.beteta@hw.ac.uk, arne.skauge@energyresearch.no, k.sorbie@hw.ac.uk

When viscous dominated fluid -> fluid displacements in a porous medium take place, and the viscosity of the displacing fluid is significantly lower than that of the displaced fluid, then an instability occurs known as viscous fingering (VF). The 2 fluids may be completely miscible or immiscible but in porous media the more complex phenomenon to reproduce both experimentally and in numerical simulations is immiscible viscous fingering; e.g. when water (viscosity, mw) displaces a very viscous oil (viscosity, mo) from a porous medium; i.e. when (mo/mw) » 1.
Many publications on immiscible VF have been produced over the last few decades, the vast majority of this being theoretical/numerical. In contrast, there are only a few published studies presenting experimental results on two phase (water/viscous oil) displacements showing VF with a full dataset which can be used to test any of the proposed models or numerical simulation methods. A "full dataset"includes finger patterns, oil recoveries, watercuts and pressure profiles across the system over time (vs. PV). Such datasets have become available in the last decade from researchers in Norway giving the details of several VF water -> viscous oil displacement experiments (and tertiary polymer floods) in 2D sandstone slabs for a wide range of viscosity ratios, (mo/mw) ~ 10 –7000.
Even before the above data was available, there have been many attempts to simulate immiscible VF by direct numerical simulation; i.e. solving the PDEs of 2 phase flow directly. Virtually all of this work produced some evidence of numerical instability and weak fingering, but the results did not resemble the highly ramified structure of observed experimental immiscible fingering. Many researchers identified the problem as being due to the inadequate numerics; i.e. current numerical methods for solving the transport equation did not capture the details of fingering due to numerical errors, e.g. numerical dispersion. Others, including the present authors, believed that the lack of finger resolution was not in the numerics but in the physics and in the "approach"to the problem. This was demonstrated in a paper in 2020 which showed that by starting from the fractional flow function as the principal input (fw*) and then choosing the relative permeabilities (kro and krw) such that the total mobility was maximized, very good resolved immiscible fingering could be obtained. In 3 further papers, this method was applied directly to the published immiscible VF experiments described above, and very good to excellent agreement was found for all the modelled quantities (finger patterns, oil recoveries, watercuts and pressure drops). Furthermore, the method without further adjustment could also predict the results for the tertiary polymer floods carried out after the waterfloods.
This talk will present a review and summary of these results and will present new extended results of this approach to include (1) the effects of capillary pressure; (ii) the scaling of how viscous fingering interacts with gravity (varying the viscous /gravity scaling group), and (iii) how the method has been upscaled to model waterflooding and polymer flooding in the field.

Participation:

In-Person

References:

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Poster / 122

Interfacial instability on dewetting in a capillary tube: from gradient to complex geometry

Author: Si Suo[1]

Co-author: Shervin Bagheri [1]

[1] *KTH*

Corresponding Authors: shervin@mech.kth.se, ssuo@kth.se

The displacement of one wetting fluid by another immiscible fluid, i.e., dewetting, in a confined geometry is an essential process in many engineering practices, including enhanced oil recovery, NAPL removal, and microfluidics. For dewetting in uniform tubes, the fluid-fluid interface loses stability once the dewetting velocity attains a threshold and a liquid film is entrained. In this work, we study this stability transition in complex capillary tubes with an emphasis on the geometry effects. We investigate the interfacial evolution in gradient tubes including expanding and contracting ones using phase-field simulations and lubrication theory. The results suggest that unlike in uniform tubes, the film entrainment could be suppressed due to the expanding geometry even though the capillary number once reaches or go beyond the critical value. We further numerically and experimentally investigate the dewetting processes in a necking tube with a parabolic profile, i.e., contracting first and then expanding. Three dewetting patterns are observed including stable displacement, phase trapping, and pinch-off bubbling, which depends on the capillary number and wall wettability.

Participation:

In-Person

References:

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MS06-A / 123

New insights into the mechanisms leading to the formation of localised pathways in water-saturated clayey geomaterials exposed to pressurised non-wetting fluid emulating supercritical CO2

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The successful deployment of carbon dioxide (CO2) geological sequestration in porous media is reliant on the sealing efficiency of the overlying clay-rich caprock to act as a physical barrier. Clay-rich caprock formations are considered as favourable materials to act as a seal due to them characteristically consisting of small pores providing high capillary entry pressures, hence preventing the intrusion of a non-wetting fluid (e.g., CO2).

In relation to CO2 sequestration, past experimental campaigns have traditionally focused on determining the capillary breakthrough pressure of caprock geomaterials. Only until recently have experimental results demonstrated that CO2 breakthrough is dominated by the creation of very localised channels (e.g., cracks) across the sealing barrier (Espinoza & Santamarina, 2010; Harrington et al., 2012; Busch et al., 2016 and Gonzalez-Blanco & Romero, 2022). The underlying hypothesis of this experimental work is that pore size heterogeneity governs the micro-mechanisms that ultimately control crack formation and thus, eventually, CO2 breakthrough. Therefore, this experimental campaign aims to provide evidence at the micro-scale to develop our understanding of the micro-mechanisms that lead to (or underly) the formation of large, localised channels (e.g., cracks) that pressurised CO2 is generating, causing an early breakthrough. An innovative experimental set-up which allowed for the onset of surface crack formation to be captured during gas injection into clayey geomaterials is presented. Post-mortem assessment of the aperture, volume and internal nature of these localised pathways was then visualised using the non-invasive and non-destructive xCT imaging technique.

Preliminary data on different cracking patterns when non-wetting gas (i.e., air) is injected into consolidated clay show the formation of large cracks that nucleate from the centre of the sample. Upon air pressurisation, before crack formation, the sample undergoes volumetric deformation, as the resulting action of the vertical stress applied at the air-water interface (menisci). Once a crack forms, volumetric deformation stops, and breakthrough occurs. Changing the particle size distribution, by using clay-silt mixtures, shows the potential effect of pore size heterogeneity on breakthrough and cracking patterns. Clay-silt mixtures with higher silt mass fraction result in earlier and larger crack formation, subsequently lowering the breakthrough pressure. This is opposed to the uniform pore size distribution of clay and silt materials alone, which display smaller cracking patterns. Our results, therefore, indicate that heterogeneity at the particle and subsequent pore-scale is a controlling parameter in the formation of localised pathways (e.g., cracks) in clayey geomaterials. Gas invasion into the tested clayey geomaterials occurred at lower pressures than the expected air-entry-values traditionally recorded throughout the literature. The mechanisms of air intrusion are expected to be of a similar nature as CO2 intrusion. Understanding the parameters which control the formation of localised pathways is therefore paramount when assessing the security of a geological CO2 reservoir.

Participation:

In-Person

References:

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MS06-A / 124

Multiphase flow dynamics effect on microscale phase configuration

Authors: Ilan Ben-Noah[1]; Juan J. Hidalgo[2]; Joaquin Jimenez-Martinez[3]; Yves Méheust[4]; Marco Dentz[1]

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We study the dynamics of pore-scale gas and liquid flow through a horizontal quasi-two dimensional millifluidic device. The multiphase flow dynamics is controlled by the physical properties of the fluid phases and their initial spatial distribution; it govern their spatial distribution at subsequent times, through the interplay between capillary and viscous forces. In turn, this spatial configuration of fluid phases significantly affects the relative hydraulic properties of the domain, such as conductance and tortuosity. During flow in multiphase systems, the flow rates and the phases saturation are strongly coupled. Disentangling the decoupled effect of each of these mechanisms on the phases' configuration is a major step towards the prediction of complex multiphase flow and capillary non-equilibrium conditions.

Here, we use experimental data gathered from several multiphase flow experiments conducted in a millifluidic device and using different flow dynamics (flow rates, air/liquid injection duty cycles, initial saturation degree, etc.). This data is analyzed in terms of criteria such as the water-filled pore size distribution, coordination number distribution, and air mobility. This analysis draws from a newly developed image analysis method, using the distance map curvatures to locate the critical points of pore throats and bodies from binary 2D or 3D images. Moreover, direct numerical simulation of single-phase flow is used to evaluate the velocity distributions in the percolating (imbibing) liquid phase.

In this study, we show that the phases saturation is the major driver determining the spatial distribution of fluid phases. However, capillary non-equilibrium distribution prevails even at relatively low capillary number (low velocity) conditions. The divergence from capillary equilibrium phase distribution, in terms of water filled pore size distribution and coordination number, is related to the flow dynamics. In addition, we relate quantitatively the magnitudes of capillary and viscous forces to the air clusters'shape and size probability density functions, and how the liquid preferential flow evolves through the most conducting (larger pores) paths.

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MS21 / 125

Numerical Challenges in Numerical of Foam Displacements in Porous Media

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We review challenges to accurate simulation of processes of foam injection into geological formations for CO2 storage, aquifer remediation and enhanced oil recovery, with a focus on numerical issues (Rossen, 2013). Foam responds in an abrupt, nonlinear way to changes in water saturation, surfactant concentration, and oil saturation, in ways that cause fluxes to fluctuate in time and space. For instance, in simulations of foam with oil, consecutive grid blocks can lie on opposite sides of a strong foam/weak foam boundary on the composition diagram. The fluctuations can be suppressed by including capillary diffusion in the simulation. In addition, difficulty in representing shock fronts can lead to an increase in the foam-swept zone in simulations. As the grid is refined these effects have smaller impact on the overall process but execution of the simulation slows. Consideration of the 1D fractional-flow solution for the same displacement can determine whether the increase in foam sweep is a numerical artifact (Lyu et al., 2021a,b).

The representation of near-well effects on injectivity can require an impractical level of grid resolution near an injection well (Gong et al., 2020a,b). In addition, some near-well effects are not yet represented in foam simulators. An imperfect solution is to refine the grid to the extent practical and simply disregard the rise in injection-well pressure predicted by the Peaceman in the injection-well grid block.

Because by definition foam is an interaction between gas and water, the naming of phases (gas or oil) in a compositional simulation of a miscible EOR process can have significant effect on the simulation of a foam displacement. Numerical dispersion of surfactant concentration is also a problem, but attempts to minimize its effect can lead to other numerical artifacts. Because foam is so sensitive to water saturation and capillary pressure, capillary effects are important, especially in finely laminated formations.

“Population-balance” foam simulators, which represent the complex dynamics of bubble creation and destruction along with the effect of foam on gas mobility, face additional challenges with instability and slow run times, especially for models that represent the multiple steady states seen in the laboratory. A minimum velocity for foam generation in co-injection of gas and liquid can be represented by at least two simulation models (Yu and Rossen, 2022), but the implications for foam propagation may not be fully resolved.

We collect and review the various numerical challenges to foam simulation. Some of these problems

are largely cosmetic, giving for instance fluctuating fluxes and pressure gradient but no significant effect on sweep and final recovery. Others do severely influence the whole progress of the flood. We discuss the origin of the challenges, how to recognize them, how they can be mitigated, and whether they arise from a correct representation of foam physics or the unintended result of attempts to solve other numerical problems.

Participation:

In-Person

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Investigation of foam evolution in fractured-vuggy reservoirs

Authors: Zhengxiao Xu[1]; Zhaomin Li[2]; Lei Tao[1]; Tong Yu[3]; Zihan Gu[2]

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For deep fractured-vuggy carbonate reservoirs, foam flooding is an effective oil recovery method. However, the harsh formation environment (high temperature, high pressure, high salinity, etc.) affects the stability of foam. Therefore, it is necessary to conduct a comprehensive investigation on the migration characteristics of foam, in order to provide guidance for the oilfield application of foam flooding.
A visual experimental model with characteristics of fractures and caverns was built in this work. The dynamic and static processes of foam in visual models were recorded by camera, and the flow and structural evolution of foam were analyzed. At the same time, the corresponding fracture and cavern model was established by simulation software, and the flow and evolution process of the foam

were simulated. The factors such as interfacial tension and liquid viscosity were adjusted, and the matching relationship between foam and fractures was considered. The characteristics of the foam migration in fractured-vuggy reservoir were summarized.
The experimental results show that in the oil recovery process of fractured-vuggy carbonate reservoirs, injected water mainly displaces the bottom crude oil, injected gas mainly displaces the top crude oil, and foam flooding can adjust the displacement profile and increase the oil washing efficiency. When foam is observed in static state, the foam in the fracture is more stable than that in the cavern, which is related to the shape and structure of the foam. The simulation results show that in the foam drainage process, as the interfacial tension between the gas and liquid phases decreases, the time to collapse of the foam liquid film increases, that is, the foam life increases. As the viscosity of the liquid phase increases, the foam stability increases. In the process of foam coalescence, the pre-bubble has a disturbing effect on the post-bubble. With the decrease of the interfacial tension and the increase of liquid viscosity, the time for the completion of the coalescence between bubbles increases.
Through the establishment of visual fractured-vuggy model can intuitively record and analyze the flow and evolution process of foam. Based on the experimental correlation characteristics, a corresponding foam flow model is established by means of experiment and simulation, and a variety of influencing factors are analyzed.

Participation:

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Poster / 127

Discontinuous Phase Flow in Porous Media: A Pore-scale Approach

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Discontinuous phase flow behavior is different from that of the continuous phase flow. In addition to that, depending on factors such as the pore structure, the wettability, the discontinuous phase can exist in many forms. Each form may exhibit a specific flow behavior. Numerous studies have been performed on the mobilization of discontinuous phases. However, many works have been performed on two-dimensional models, only few works considered in three-dimensional models. Different geometries have been also studied in literature. A complete understanding of the discontinuous phase flow requires to study a large range of parameters that affect the flow including drawing clear differences between the 2-D and 3-D approaches, the geometries, and different forms of discontinuous phases. This requires a pore-scale perspective where fluid interfaces are taken into account.

To study the discontinuous phase flow, we have performed pore-scale simulations. The phase morphology and mobilization pressure have been investigated. Research have shown that isolated droplets are one of the most difficult trapped discontinuous phase to displace. In unconstructed channels, the discontinuous phase is mainly trapped due to the surface wettability contrast. In constricted channels, the comparison of 2-D and 3-D models have shown that 3-D models capture the morphological shapes that cannot be captured in 2-D models, such as the saddle-shape in fractional-wet porous media. Furthermore, droplet dynamics in a fractionally-wet channel do not necessarily follow the same behavior as in a uniform capillary channel and cannot be predicted using uniform wettability surfaces depicted by an average contact angle. In particular, the pressure difference needed to push the droplet through the restriction with fractional wettability is lower than that for a uniform channel with a constant contact angle representing the less favorable wettability state. Due to the geometry, isolated droplets can be categorized as long droplets and finite droplets. The discrepancy in their mobilization have been studied. We have also considered a discontinuous phase spanning multiple pores. The results have shown that the existing models can not accurately capture topological changes of a ganglion.

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Flow of Liquid Through a Stagnant Foam in a Model Fracture

Authors: Ewald J. M. Obbens[1]; Kai Li[1]; William Rossen[2]

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Foam is a promising means of increasing carbon storage in CO2 sequestration projects and waste isolation and removal in soil remediation, and a proven tool for enhanced oil recovery. Many of these applications involve fractured geological formations. Li et al. (2021a) studied inter-bubble diffusion and coarsening in foam in two glass model fractures. The bubbles were larger than the gap between fracture walls, so that only one sheet of bubbles occupied the model. As part of that study, they showed how one can determine water saturation and capillary pressure in the model fracture from analysis of visual images of the foam, specifically the location of wetting liquid along the uneven aperture in the model fracture (Li et al., 2021b). This approach would not be possible in a conventional microfluidic device with uniform depth of etching. Their approach depends on an assumption that capillary pressure is uniform within the region of an image, which was (0.8 cm)^2 and (2 cm)^2 for the two model fractures.
We describe a model for the flow of water through the Plateau borders of the foam in these experiments along the top and bottom fracture surfaces. The width of the Plateau borders is determined by capillary pressure, as determined by Li et al. Numerical solution for velocity and flow rate through the Plateau borders then allows flow rate along each to be determined as a function of capillary

pressure and pressure gradient. A numerical model then solves for flow through the network of Plateau borders along the fracture wall. We allow for either no-slip or zero-shear-stress boundary conditions at the water-gas interface, reflecting the two extremes of foaming surfactant behavior. Our results show that water redistributes itself to equalize capillary pressure across the image area in the order of tens of seconds. Thus the assumption of Li et al. (2021b) is justified. The relative permeability of water through the Plateau borders in a trapped foam in these model fractures lies between 1E-04 and 1E-07, depending on capillary pressure and bubble size. This method could also be applied to determine the relative permeability of water in trapped foam from images of the foam in conventional microfluidic devices, if one can measure or infer capillary pressure within the device.

Participation:

In-Person

References:

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Pore-scale Investigation of Hydrogen-Water Displacement and Trapping Mechanisms during UHS Process

Authors: Mehdi Bahrami Karkevandi[1]; Hassan Mahani[1]; Shahab Ayatollahi[1]; Davood Zivar[2]

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Hydrogen storage in porous subsurface environments, such as aquifers or depleted gas reservoirs, is a high-potential option for cyclic hydrogen storage that can balance renewable energy supply and demand on a large scale due to its high storage capacity. The main impediment to the development and widespread application of underground hydrogen storage (UHS) is the poor understanding of hydrogen flow dynamics in porous media, therefore the volume of recoverable hydrogen for this cyclic process is unclear. We employed a 2D glass micromodel and a microfluidics system and performed the drainage and imbibition cycles. The saturation achieved in each cycle was used to determine the effect of hysteresis on hydrogen trapping and the recovery factor of the hydrogen storage process. In addition, to assess the flow behavior of the hydrogen-water system, we imaged at high resolution the pore-scale displacement and trapping mechanisms that occur during imbibition. We also conducted the CO2-water system experiments at settings similar to the H2-water system tests

and compared their pore-scale fluid flow characteristics. Our observations indicate that the amount of trapped saturation of H2 and CO2 at the end of the imbibition process increases as the number of cycles increases. It is roughly 10% for the CO2-water system and 40% for the H2-water system. The dissolution of CO2 in water during imbibition is the main cause of its lower residual saturation. Furthermore, pore-scale fluid flow visualization shows that, upon initiation of the imbibition process, water disconnects the hydrogen phase and a significant volume of gas is bypassed. Hydrogen displacement is mainly achieved by piston-like throat-filling and I1 cooperative pore-filling mechanisms. The findings of this study improve our knowledge of the UHS process in porous media by revealing details about the pore-scale flow behavior of hydrogen water fluids.

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EXAMINING THE FEASIBILITY OF USING ZERO-VALENT BIMETALS FOR THE TREATMENT OF TRICHLOROETHYLENE VAPORS IN THE UNSATURATED ZONE

Author: Clarissa Settimi[1]

Co-authors: Daniela Zingaretti [1]; Iason Verginelli [1]; Renato Baciocchi [1]

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Chlorinated solvents, such as trichloroethylene (TCE), have caused groundwater and soil contamination for years due to their massive and uncontrolled use adopted in the past [1]. Once released in the subsoil, these compounds are characterized by high mobility and low biodegradability with a consequent persistence in the environment [2]. For these reasons, in most industrialized countries, groundwater bodies are currently characterized by diffuse contamination by chlorinated compounds, which can cause potential long-term risks to human health [2-4]. In particular, the most critical migration pathway for chlorinated solvents is the volatilization from the subsoil into overlying buildings (i.e. vapor intrusion) [5-6]. Traditional remediation techniques in sites characterized by diffuse contamination by chlorinated solvents are not technically and economically sustainable as they typically require significant amounts of reagents or energy [4]. In this scenario, it is thus more indicated to adopt risk management strategies aimed at interrupting the migration pathway of chlorinated solvents vapors to air ambient or into buildings [3-4]. Recently, it was proposed to use horizontal permeable reactive barriers (HPRBS) placed in the unsaturated zone to treat upward volatile organic compounds vapors [3-5, 7-8]. Zero-valent iron (ZVI) was proposed as reactive

material for HPRBs and tested for TCE degradation in the vapor phase through reductive dehalogenation [3-4]. In the last years, ZVI bimetals have also been widely studied for the enhancement of the degradation of chlorinated compounds via iron corrosion or hydrogenation in contaminated groundwater [9-11]. However, such bimetals were poorly investigated to treat chlorinated solvents in the vapor phase [12-13]. In this study, we examine the feasibility of using zero-valent Fe-Cu ad Fe-Ni bimetals for the degradation of TCE vapors at partially saturated conditions. Different bimetals were synthesized by mixing Fe and Ni or Cu powders using disc milling and then characterized. The produced bimetals were then tested in anaerobic batch TCE vapors degradation tests at different reaction times to evaluate their reactivity towards dechlorination. The disc-milled bimetals produced were characterized by a homogenous distribution of Ni or Cu in the Fe phase and micrometric size. In all the experiments, complete degradation of TCE vapors was achieved in maximum 4 days with zero-order degradation kinetics. Fe-Ni bimetals have shown better performances in terms of TCE removal than Fe-Cu bimetals leading to a complete degradation of TCE in the vapor phase after 2 days of reaction. These results showed a significant enhancement in TCE removal compared to ZVI alone, which was found to entirely degrade TCE vapors after minimum 2 weeks of reaction in previous studies [3-4]. The only detectable reaction byproducts in the tested conditions were C3–C6 hydrocarbons. No vinyl chloride (VC) or dichloroethylene (DCE) peaks were observed. In view of using the tested bimetals in HPRBs to treat chlorinated solvent vapors emitted from contaminated groundwater, the experimental results obtained were integrated into an analytical model to simulate the reactive transport of vapors through the barrier. It was found that an HPRB of 20 cm could ensure a complete reduction of TCE vapors.

Participation:

In-Person

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Pore-scale Simulation of the Effect of Interfacial Viscoelasticity in Low-Salinity Waterflooding

Authors: Ahmadreza Kamani[1]; Shahab Ayatollahi[1]; Hassan Mahani[1]

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The study of fluid-fluid interfaces is an interesting research topic, especially for multiphase flow in porous media. During oil recovery by waterflooding, the fluid-fluid interface exhibits a complex rheological response to deformations which affects the wetting and not-wetting phase trapping. For structured interfaces, the simple isotropic interfacial tension does not completely describe the interfacial response to deformation, hence interfacial constitutive relations must be defined to achieve this goal. Depending on the complexity of the oil, brine, and rock, different amounts of oil are trapped underground after primary and secondary recovery stages. Therefore, it is necessary to use enhanced oil recovery techniques to maximize oil recovery efficiency.

Low-salinity waterflooding has proved to be technically and environmentally feasible. Recent studies have shown the sensitivity of the interfacial properties of reservoir fluids to the type and amounts of macromolecules (such as asphaltenes) as they are populated and structured at the interface by electrostatic attractions. The inhomogeneous distribution of macromolecules at the interface leads to an interfacial tension gradient and this heterogeneity causes isotropic (dilatational) and deviatoric (shear) stresses. The inherent complexity of displacement by low-salinity waterflooding, necessitates investigation of the effect of interfacial dilatational and shear stresses (interfacial rheology) at the pore-scale. Interfacial properties at the pore-scale would affect phase connectivity, snap-off, stability of droplets, fingering, and wetting/de-wetting dynamics.

In this research, we investigated the effect of low-salinity water on the trapping of the non-wetting phase caused by the snap-off process, as the most well-known type of microscopic trapping in porous media. A water-wet porous medium containing two Newtonian fluids under capillary pressure effect with viscoelastic interface was selected to study the rheological constitutive models. Computational fluid dynamics simulations were performed with OpenFOAM (Open-source Field Operation And Manipulation). To solve the two-phase flow with a complex interface, interFoam solver of OpenFOAM was extended. A parametric study was performed assuming that maximum elasticity occurs in the low-salinity water phase surrounding an oil ganglion as the non-wetting phase in the pore-scale model.

The results show that the effects of dilatational viscoelasticity lead to expansion/compression of the interface with changes in the interfacial area and the effects of shear viscoelasticity lead to changes in the interfacial shape. Depending on the rheological properties of the interface and geometry of the porous medium, these effects make the oil phase remain continuous and improve recovery. Although increasing the elasticity of the interface reduces the probability of instability and the breakup of the oil ganglion, it may reduce the oil production rate through narrow throats. Moreover, the presence of angular corners in the geometry intensifies these effects.

The novelty of this work is the modeling of the multiphase fluid flow with a viscoelastic interface. Since laboratory results may not be accurate due to the difficulties in performing experiments on the interface, modeling the interfacial viscoelasticity seems to be a good solution for the prediction of the fluid flow with a viscoelastic interface.

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MS15 / 134

Introducing Barlow Twins deep operator networks as a proxy for geologic carbon storage

Authors: Teeratorn Kadeethum[1]; Nikolaos Bouklas[2]; Somdatta Goswami[3]; George Karniadakis[3]; Hongkyu Yoon[1]

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Geologic carbon storage (GCS) is a viable technology that can reduce carbon emissions to the atmosphere and mitigate the impact of climate change. Undeniably, a better understanding of the seismic potential in a GCS site and developing a corresponding mitigation strategy for risk management plan is required to ensure operational safety and minimize environmental impacts. To achieve this, a fast surrogate model is very powerful since many geological structures and operating conditions must be evaluated for their sensitivity and uncertainty in model prediction, while maintaining an acceptable accuracy level of high-fidelity models. In this work, we present Barlow Twins deep operator networks to be used as a surrogate for geologic carbon storage, with application for the Illinois Basin Decatur Project (IBDP) site, where a million metric tonnes of CO2 have been injected. The proposed data-driven framework is built upon a combination of deep operator networks (DeepONets) [1], and Barlow Twins reduced order models (BT-ROM) as well as its variations [2, 3]. To elaborate on this, we use DeepONets' architecture of branch and trunk nets in combination with a projector from BT-ROM. The loss function is constituted of point-wise differences (mean squared errors) and redundancy reduction terms. Our goal is to enhance DeepONets' capability by achieving better-reduced manifolds through an information bottleneck principle and a joint embedding architecture of BT-ROM. Our parameter space (input) contains heterogeneous hydrogeological properties (permeability and porosity) and operation constraints (e.g., varying injection rates and bottom hole pressure). We will compare a surrogate model performance with a high fidelity model in terms of fluid pressure and CO2 saturation.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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135

Pore-Scale Simulation of the Interdependency of the Corner-Flow, Roughness, and Time-Effect on the Efficiency of Low-Salinity Waterflooding in a Mixed-Wet System

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Low-salinity waterflooding (LSWF) is a promising EOR approach that decreases the oil-wetness of reservoir rocks, hence increasing the recovery factor. The efficiency of LSWF depends on the initial wettability of the system. All conventional oil reservoirs are formed by oil migration during primary drainage. During the drainage phase, the reservoir brines in the corners of pores cannot be displaced by oil due to very high capillary pressure; thereby rendering a mixed-wet system. Corner flow in mixed-wet systems, based on the pore distribution and fluid location may provoke positive and negative effects during LSWF. In this study, we have evaluated the effect of corner flow and surface heterogeneities (roughness) on the efficiency of secondary mode LSWF by direct numerical simulations using OpenFOAM (Open Source Field Operation and Manipulation) in 2D and 3D pore-scale models.

The simulation results show that LS water can move ahead of the oil phase through the corners, thus wettability alteration may occur in front of the oil-water interface located in the center of the pores leading to a faster oil relocation, oil snap-off entrapment and blockage of the oil production path. Besides, during secondary LSWF, an interplay between corner flow and surface heterogeneities is observed, through which the LS water that is moving in the corners would alter the wettability of the oil-wet surfaces. This phenomenon show the effect of surface heterogeneities in our geometries, which may either increase or decrease the residual oil saturation, depending on the kinetics of wettability alteration. Simulations in a 2D model without corner flow show that in some cases the recovery factor can increase by 18%, indicating the adverse effect of corner flow in our geometries. Simulations in the same pore geometry but with surface roughness show a decrease in the

displacement sweep efficiency compared with a system consisting of smooth pore surfaces wherein the effect of corner flow was not taken into account.
The results of this research show a more realistic output of the two-phase flow behavior due to incorporating various aspects of pore-geometry into our model and also highlight that the interplay between the aforementioned phenomena and the time dependency of wettability alteration (kinetics) may adversely affect the LS injection efficiency.

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Poster / 136

ASSESSMENT OF THE ACCURACY OF THE SOIL GAS RADON DEFICIT TECHNIQUE FOR MONITORING AND QUANTIFYING RESIDUAL LNAPL CONTAMINATION

Author: Alessandra Cecconi[1]

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Hydrocarbon spills into the subsurface can lead to the formation of light non-aqueous phase liquids (LNAPL), i.e., a separate phase, immiscible with water, representing a long-term environmental threat. Traditionally, the presence of mobile LNAPL is evaluated by installing monitoring wells in the area of potential concern [1]. This approach, however, provides only qualitative evidence of the thickness of LNAPL observed in the wells, thus not providing information on the distribution of residual LNAPL in the subsurface [2].
As an alternative, in the last decades, radon (Rn) has been widely proposed as a naturally occurring tracer for light non-aqueous phase liquids in the soil (e.g., [3], [4]) since it has been shown to tend to partition into LNAPL. Rn concentration in soil gas is expected to decrease in the impacted area compared to the value observed at background locations (not impacted by LNAPL), creating a measurable Rn deficit. This work examines the feasibility of using soil gas data collected in unsaturated soil at some distance from the source zone to apply the Rn deficit technique to identify and quantify LNAPL contamination. To this end, we developed a steady-state 1-D analytical solution based on a 3-layer model that simulates the transport and distribution of Rn in the source zone, capillary fringe, and overlying unsaturated soil [5]. The analytical solution was first validated against a more detailed numerical model available in the literature [6]. Then, a series of simulations were carried out to evaluate the vertical concentration profiles of Rn in soil gas above the source zone and in a background location not impacted by LNAPL. Simulation results showed that the parameters that most influence the migration and distribution of Rn in the subsurface are the distance of the soil gas probe from

the source zone and, to a lower extent, the type of contamination (e.g., diesel or gasoline) and soil type. Based on these results, to aid the determination of LNAPL saturation, some nomograms have been developed that can be used to apply the Rn-deficit technique from Rn concentration data in soil gas collected at a certain distance from the LNAPL source zone. The developed nomograms show that the Rn deficit is more evident as the measurement point approaches the source area. According to the obtained results, the Rn deficit technique is a feasible method for qualitatively identifying residual LNAPL when Rn in soil gas is measured at distances lower than 2m from the contaminated zone. However, for an accurate quantitative estimation of the LNAPL phase content, soil gas probes should preferably be located at distances lower than 1m from the source zone.
The nomographs provided in this work, which allow the estimation of LNAPL saturation as a function of the distance of soil gas probes from the LNAPL source zone and of the type of soil and contamination, are generally applicable to all sites involving relatively homogenous soils. Conversely, more sophisticated numerical models should be preferred (e.g., [6]) in the case of heterogeneous soils involving geological barriers or stratified contaminations.

Participation:

In-Person

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MS08 / **137**

Dynamics of microplastic fiber mobility in a periodic porous media: Experimental results and numerical simulations

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Microplastic fibers (MPFs) are the largest kind of microplastic in the environment by mass and their presence has been identified on every continent and ecosystem on the planet. MPFs are known to

pose a threat to aquatic species and worms but impacts on larger animals and humans are largely speculative, in no small part to the difficulty in quantifying the dynamics of how these non-dissolved, colloidal masses move. The objective of this work was to advance our basic knowledge regarding how simple kinds of MPFs move through porous media using a combination of experimentation and numerical simulation. Pseudo-2d flow chambers, termed "meso-models,"were created as oversized analogs of micro-models that were big enough to inject fibers into a controlled flow field. High fluorescence MPFs were injected into the flow between an opaque backing and a clear polycarbonate top sheet, the flow was subjected to UV light, and the MPF paths through the periodic pore meso-model were captured directly using HD video. Image processing extracted the trajectories providing position and time from which both breakthrough curves and velocity statistics could be extracted. Numerical simulations of the experiments using the known pressure gradients and flow rates from the experiments were constructed and a bead-rod chain model of MPF migration [1] was tested against the experimental results. The numerical and experimental results showed strong similarities, differing mainly by variations that can likely be attributed stochastic fluctuations. These results are the first direct capture of MPF dynamics in any porous media and the encouraging agreement with the numerical results suggests that, despite their extraordinary complexity, predictive modeling of MPF dynamics is feasible, which will be essential for realistic risk assessment of any direct or indirect hazards posed by MPFs.

Participation:

In-Person

References:

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Poster / 139

A Macroscopic Model for Unsaturated Flow in Deformable Evolving Porous Media

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In this work we derive a model for a deformable porous medium with a growing interface and with phase change to model eco-hydro-mechanical problems in which there is a continuous deposition of porous substrate on the surface and the simultaneous decay and phase change between solid and fluid. The model will then be simplified for one-dimensional scenarios or in multi-dimension under small deformations, leading to a treatable set of equations. The time and length-scales of the problem are discussed and its limiting behaviour is discussed with the help of numerical simulations. Applications to environmental and manufacturing problems are discussed.

Participation:

In-Person

References:

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Poster / 140

Enhancing a high-fidelity nonlinear solver with reduced order model for induced seismicity

Authors: Teeratorn Kadeethum[1]; Kyung Won Chang[1]; Austin A. Holland[1]; Hongkyu Yoon[1]

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Even though geologic carbon storage could reduce carbon emissions to the atmosphere and mitigate the impact of climate change, there are potential seismic risks and uncertainties associated with a GCS operation. Hence, we need to understand this process better before it becomes a reliable technology. However, the system of partial differential equations used to describe an induced seismicity event is highly nonlinear. Subsequently, we need substantial computational resources to approximate this system, making this process unsuitable for handling large-scale uncertainty quantification in which an extensive set of simulations must be explored. Kadeethum et al. [1] have illustrated the use of reduced order modeling (ROM) to enhance full order modeling (FOM) solvers. In this study, we apply the framework to an induced seismicity high-fidelity solver (coupled hydro-mechanical (HM) processes) proposed by Chang et al. [2]. Our goal is to investigate the improvements of ROM-assisted FOM performance with emphasis on (1) computational cost reduction and (2) a convergence rate. Our systematic approach is:
1. Substitute the high-fidelity hydro (H-FOM) solver with the low-fidelity hydro (H-ROM) model but still use high-fidelity mechanics (M-FOM) solver: H-ROM-M-FOM.
2. Substitute the M-FOM solver with low-fidelity mechanics (M-ROM) model: H-FOM-M-ROM.
3. Use HM-FOM with HM-ROM initialization.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS10 / 141

Integration of SEM Images and NMR Measurements to Characterize Pore Size Distributions in Unconventional Tight Rock Reservoirs

Authors: Paul Hart[1]; Elton Yang[1]

Co-author: Luisa Crousse [1]

[1] *Chevron*

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Pore size distribution (PSD) is a key parameter in Shale & Tight (S&T) reservoir evaluation, significantly contributing to our understanding of storage capacity and distribution / producibility of reservoir fluids. We have taken a collaborative approach to develop a new workflow for evaluation of PSD through the integration of (lab-based) 2D Scanning Electron Microscopy (SEM) and Nuclear Magnetic Resonance (NMR) T2 distributions. Our method uses large area SEM imaging and incorporates data from two different detectors to improve statistics of PSD. Application of this workflow on a variety of S&T formation samples has demonstrated promising results, enabling downhole in-situ PSD estimation for an entire NMR logged wellbore interval. This new technique has the potential to yield several impactful outcomes including improved understanding of in-situ PSD, faster / enhanced petrophysical evaluation, and improved forecasting of resource production.

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Poster / 142

Investigation of supercritical CO2 mass transfer in porous media using X-ray micro-computed tomography

Author: Ruotong Huang[None]

Co-authors: Anna Herring [1]; Adrian Sheppard [2]

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Understanding the mass transfer of CO_2 into formation brine both qualitatively and quantitatively is important for improving the security of geologic carbon sequestration. In this study, quasi-dynamic X-ray micro-computed tomographic (MCT) imaging was used to track the time-evolution of supercritical CO_2 ($scCO_2$) clusters in a sandstone throughout brine injection. A cluster-matching workflow enabled the identification of depletion, merging, and snap-off of the $scCO_2$ clusters, and subsequently the mass transfer coefficient of individual $scCO_2$ clusters was found to range between 3.0×10^{-5} and 3.5×10^{-4} mm/s. The macroscopic average mass transfer coefficient was estimated as 1.4×10^{-4} mm/s. For application to geologic carbon sequestration, these values give an indication of the range of mass transfer coefficients that may be expected for similar state and flow conditions. With the macroscopic average mass transfer coefficient evaluated, we back-calculated the *in-situ* CO_2 concentration field for brine, which provides quantitative insight of the distribution of dissolved CO_2 in the sample. Despite slow injection rate (Ca = 10^{-7}), mobilization of small $scCO_2$ clusters was also observed, and was attributed to the combined effect of incomplete dissolution of snapped-off clusters and the reduction in the fluid–fluid interfacial tension (IFT) due to the high local CO_2 concentration in brine accompanying $scCO_2$ dissolution. This highlights the coupling of dissolution and mobilization processes and demonstrates the need to understand these interlinked dynamics to improve CO_2 storage in geological formations.

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Energy Transition Focused Abstracts:

143

An Integrated Approach to Evaluate Lacustrine Shale Oil Reservoir Combining Advanced Well Logging and Core Analysis

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Unconventional reservoir is a hot spot worldwide. With the high demand of oil and gas in China, the exploration and development of unconventional reservoirs maintains in a high level. In order to evaluate the lithologies, pore structures, porosities, TOC in quantities accurately. The advanced gamma ray spectroscopy logs, 2D nuclear magnetic resonance (NMR) logs, and high-resolution micro-resistivity borehole image logs were acquired in some key wells. Integrated with core data like XRD, MICP etc., the lithofacies together with rock texture were classified based on the minerals from gamma ray spectroscopy, borehole image, The physical properties, pore size and fluid distribution was interpretated with 2D NMR toghther. The combination of these three facies represents the reservoir quality. TOC from spectroscopy and oil volume from 2D NMR helps define the TOC from Kerogen, then the source rock quality is further evaluated.

In the study area, the lithofacies were classified into four types, which are Calcite dolomite facies, Dolomite calcite facies, shale facies and sand facies. The textures were classified into two types, thin-layer and laminate. Thus, there was a cross-assignment to make the final reservoir facies to seven different types. With the investigation and summarization, The pay zone of the reservoir and source rock quality were well defined and mapped vertically and horizontally in the whole study area. The relationship for source rock and reservoir quality is further defined based on the analysis above.

The integrated approach described in this study leverages the advantages of the advanced gamma ray spectroscopy, NMR, borehole images and core measurements. It develops the comprehensive understanding of the complex carbonate reservoir and provide the solution to define source- reservoir relationship, get the sweet spots and place the horizontal well.

This integrated workflow provided understanding and solutions in different scale and this input was crucial for further geological study in the area. The integrated workflow has already led an example to evaluate lacustrine shale oil reservoir which now spread to other integrated studies in Qadam basin and other oilfields.

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Energy Transition Focused Abstracts:

MS21 / **144**

Inertial solution for high-pressure-difference pulse decay measurement through microporous media

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We present a theoretical asymptotic solution for high-speed transient flow through micro-porous media in this work by considering the inertia effect in the high-pressure-difference pulse decay process. It includes all three gas related effects, that are the inertia effect, the slippage effect, and the compressibility effect. Capillaric model, in which a bundle of straight circular tubes whose radius is much smaller than length is used to represent the internal structure, is adopted and the flow is described by the unsteady-state incompressible Navier-Stokes equation with mean density in two-dimensional case, capturing the main characteristic of mass flow rate. By order of magnitude analysis and asymptotic perturbation, our inertial solution along with its dimensionless criterion for high-pressure-difference pulse are derived. The theoretical results are verified using our self-built experimental platform, by comparing the permeabilities calculated by our inertial solution and the benchmark steady-state measurement. Our inertial solution can shorten the measurement time and is expected to be used in measurement of extremely low-permeability samples.

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MS17 / 146

Simulation Study of In-situ Conversion Process in Low-mid Maturity Shale Oil Reservoir

Author: Zijie Wang[1]

Co-authors: Jun Yao [2]; Hai Sun [1]; Xia Yan

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Continental shale oil in China is mainly of low-medium maturity, filled with heavy oil of low mobility and organic matter that unconverted. Horizontal drilling and hydraulic fracturing are insufficient to obtain economic production in such reservoir, thus in-situ heating and transform technology should be applied. A multiphase multicomponent hydro-thermal coupled numerical model considering multistage kinetic reactions is developed to describe the decomposition of solid organic matter, cracking of heavy hydrocarbon, phase behavior and rock property evolution.
During the in-situ process, organic matter (kerogen) decomposition and heavy oil cracking happens, enhancing hydrocarbon mobility. The research focuses on the development of multiphase multicomponent hydro-thermal coupled numerical model, with the evolution of porosity and permeability

considered. The finite volume method is used for the space discretization of flow and heat transfer equation, and solved by the fully coupling method. Finally, the impact of important parameters on cumulative production are analyzed.
The compositional flow model is validated by comparing the results with those of CMG, and the coupled hydro-thermal model is validated against COMSOL Multiphysics. The impact of parameters including heating temperature, kerogen concentration, well bottom hole pressure, heater pattern and initial water saturation on cumulative production is analyzed. The results are summarized as: kinetic reaction rate is controlled by temperature and different reactions take place at variety heating temperature, influencing the fluid composition; higher kerogen concentration can enhance cumulative hydrocarbon production after in-situ conversion, making it an important parameter to evaluate before production; low bottom hole pressure can extract hydrocarbon products in time to prevent from further cracking and coking; different heater pattern has impact on the ratio of energy output to energy input, and hexagon heater is the most benefit; high water saturation will enhance energy consumption to heat water and reduce the utility ratio of energy, thus dewater process is required to reduce water saturation. It can be concluded that the in-situ conversion process is feasible in low-mid maturity shale oil reservoir, during which kerogen decomposition and hydrocarbon cracking happens. Besides, the operating parameters should be investigated to make the heating process economical.
The proposed model provides an efficient tool for modeling the in-situ conversion process of low-mid maturity shale oil reservoirs. In this paper, the reservoir fluid property variation, in-situ porosity and permeability evolution, and production characteristics are illustrated, which could provide insights on heater design and well operational management. With multiple transport mechanisms and multi stage kinetic reactions incorporated, the hydrocarbon production characteristics and formation property evolution of shale reservoirs can be both accurately captured.

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MS01 / 147

3D X-Ray Visualization of Rayleigh-Bénard Instability in a Porous Medium

Author: Sotheavuth Sin[1]

Co-authors: Shun Imai [1]; Shintaro Matsushita [1]; Tetsuya Suekane [1]

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In geological storage of carbon dioxide (CO2), CO2 captured from large emission sources, such as thermal power plants, is injected into the brine-saturated reservoir under a supercritical condition

with a density of 600-700 kg/m3. One of the primary concerns in geological storage is the leakage of CO2 due to buoyancy force. The dissolution of CO2 into formation brine improves CO2 storage security. Because natural convection between CO2-saturated and CO2-free brines governs the dissolution processes, many works have been reported on the onset of natural convection and its mass transfer using Rayleigh-Bénard convection. In this work, we report a three-dimensional (3D) experimental investigation on the onset of Rayleigh-Bénard convection in a porous medium and its mass transfer. A packed bed with plastic particles saturated with water was used as a 3D porous medium. In contrast, alkaline acid soap containing sodium iodide (NaI) was used for the top boundary to model the dissolution from a rigid solid surface. The dissolution of alkaline acid soap into water forms an unstable density profile, triggering Rayleigh-Bénard instability in a porous medium. The fingering structures of Rayleigh-Bénard convection were visualized by using the X-Ray micro-computed tomography scanner (X-Ray CT). The experimental conditions cover the Rayleigh number (Ra) range between 2700 and 8100. Because the critical wavelength decreases with an increase in Ra, the finer fingers appear on the top boundary for the higher Ra. The fingers merged into the large fingers, which extended vertically downward with time. The onset time of convection reduces with Ra, and the mass transfer increases with it. These results are compared with the previous numerical works. Finally, we discuss the appropriate modeling of natural convection in geological storage.

Keywords: 3D X-Ray Visualization, Fingering Structures, Rayleigh-Bénard Instability, Rayleigh number (Ra), Natural Convection.
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Participation:

In-Person

References:

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MS10 / **149**

In-situ visualisation of microbial hydrogen consumption using high-resolution PET-MRI

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The efficiency of short and long term underground hydrogen storage in subsurface porous media is one of the limiting technical challenges facing the renewable energy industry. Storage and withdrawal efficiency may depend on microbial consumption of molecular hydrogen promoted by conducive environmental and physical conditions in the porous medium that favour growth and survival of many anaerobic microorganisms. Relevant to UHS are bacteria and archaea. The organisms depend on molecular hydrogen as an electron source for cellular respiration. In this study, state-of-the art visualization techniques were utilized to study hydrogen consumption and bacteria growth in 6 cm x 1.5 cm sand and glass bead packs. A multi-modal magnetic resonance imaging (MRI) - positron emission tomography (PET) scanner was used to study both static and dynamic phenomena, respectively. Sand and glass bead packs were saturated with bacteria solution (a sulphate-reducer olei desulfovibrio alaskensis), both without and in the presence of hydrogen. The whole experiment was conducted under anaerobic conditions for the bacteria to survive and grow. In-situ visualization provided insight into the dynamics of bacterial growth and hydrogen consumption rates: MRI provided information on the spatial fluid saturation at micrometer scale. PET provided fluid displacement dynamics during injection of brine, nutrients and bacteria at high temporal resolutions. We, hence, observed bacterial growth and fluid flow redistribution at resolutions not previously used to study these phenomena at the core scale.

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MS15 / 150

Prediction of CO2 adsorption potential on coal using various machine learning techniques for CCUS application in coal formation

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Carbon Capture, Utilization, and Sequestration (CCUS) technology is recognized as a pivotal solution to reduce carbon emissions to the atmosphere and address the issue of global warming. CO2 injection in coal formations has been commonly applied to enhance methane (CH4) recovery from coalbeds and carbon sequestration in underground formations for environmental purposes. The performance of the CO2 storage and CH4 recovery process is mainly governed by the adsorption potential of CO2 against CH4 on the surface of the coalbeds. Adsorption isotherms can be measured using different experimental techniques such as volumetric and gravimetric; however, such measurements are time-consuming, expensive, and mostly irreproducible. Additionally, mathematical models such as Langmuir and Freundlich can be inaccurate, have no saturation limits, and are subject to the accuracy of the experimental work. Therefore, the present work applied a variety of machine learning (ML) techniques to predict CO2 adsorption in coal formations.

A dataset of 1,065 points was collected for different coal samples at different operating conditions. Different ML tools were applied to these data, including random forests (RF), gradient boost regression (GBR), decision tree regression (DT), and artificial neural network (ANN). The applied ML tools predict CO2 adsorption as a function of coal's properties, testing pressure, and temperature. The coal composition is based on proximate measurements that define moisture, ash, volatile matter, and fixed carbon content in the coal samples. In addition, the Vitrinite reflectance of the coal samples was used as an indicator for the coal rank. The training-to-testing data set ratio was 70:30. Typically, a set of data hidden from the model was used for the validation purpose of the predictive models.

The ML models could accurately predict CO2 adsorption of various coal properties and at different system operating conditions. The correlation coefficient (R-value) and the AAPE (average absolute percentage error) were used to evaluate the models' performance. Overall, the R-values between actual and estimated from the different ML models were all above 0.98 using training and testing datasets, with AAPE values of 6%, 8%, 12%, and 13% for DT, RF, GBR, and ANN, respectively. Sensitivity analysis depicted a high dependency of the adsorption estimates on volatile matter content, maximum vitrinite reflectance, and operation conditions.

This work demonstrates the capability of sophisticated ML tools to accurately estimate the CO2 adsorption on the surface of coalbeds as a function of coal properties and testing pressure and temperature without the need for experimental measurements or complicated calculations.

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MS05 / **151**

Systematic screening of microbial induced calcite precipitation kinetics via online monitoring

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Microbial urease catalyses the hydrolysis of urea to ammonium and carbonate, which results in an increase of the environmental pH value. Addition of calcium ions then leads to calcium carbonate precipitation. Microbial Induced Calcite Precipitation (MICP) is successfully applied for, e.g., restoration of construction materials, soil reinforcement, or metal and radionuclide bioremediation. However, the precipitation process requires further optimization to make industrial application of MICP more efficient.

A high precipitation rate of $CaCO_3$ in the pore space of consolidated sand samples is necessary to increase the compressive strength. Multiple parameters as e.g. the urea and calcium ratio and concentration have been described in literature to have an influence on the precipitation process. However, most studies do not monitor the precipitation reaction itself, but perform application experiments on sand matrices and only check for the outcome data, typically compressive strength or the calcite content. Nevertheless, a small number of studies do try to derive strategies to improve the overall MICP process by getting an insight on the calcite precipitation kinetics and/or the crystal formation. These studies can mainly be grouped in two categories; there are simple beaker experiments with frequent manual sampling, as well as more advanced microfluidic experiments. Besides other disadvantages, both experimental strategies fail to provide a high amount of data points from a large number of parallel set-ups. Therefore, only the screening of individual parameters can be evaluated and possible interactions between parameters are disregarded.

Here, a new high-throughput microplate assay is presented, enabling online monitoring of calcite precipitation kinetics with a measurement interval of only 150 seconds. This assay was realised by making use of the automated high-throughput microbioreactor BioLector, which is able to measure a backscatter signal of 48 wells of a microplate in parallel while shaking at high speeds. The backscatter signal, intended for biomass estimation, corresponds to the turbidity in each well. When bacterial suspension and a cementing solution containing urea and a calcium source are mixed, calcium carbonate forms and precipitates, causing the backscatter signal to increase over time. As multiple precipitation kinetics can be measured in parallel by this system, the influence of multiple parameters on the precipitation rate can be easily compared. Interactions of multiple parameters influencing the MICP kinetics can be described as well by applying a Fractional Factorial Design (FFD) experimental approach.

In this study, the parameters OD600, pH, urea- and calcium concentration, type of calcium salt and culture washing were analysed. Three settings, which showed distinct calcite precipitation kinetics, were chosen to be adapted for quartz sand cubes solidification experiments to find a correlation between compressive strength and the precipitation rate. The results showed that very fast as well as delayed calcite precipitation is disadvantageous to solidify samples with high compressive strength.

Overall, the microbioreactor system can be successfully used to measure increasing suspension turbidity. This enables an easy systematic screening of a multitude of parameters influencing the precipitation rate and could help to optimize MICP applications, e.g. for building restoration to improve porous or deteriorated building components.

Participation:

In-Person

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Poster / 153

Quick Clay: A novel alternative for well decommissioning

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At the end of a production well's life cycle, the facility must be shut down and prepared for decommissioning. This process ensures that the well site is properly sealed to prevent the migration and emission of remnant hydrocarbons that may reside within the well. This procedure is known as plug and abandonment and sees the emplacement of a series of cement-based plugs to act as this sealing mechanism. This process is also closely followed during carbon-capture-and-storage (CCS) procedures, where at the conclusion of CO2 injection into the reservoir stores, the site must be reliably sealed to prevent the extrusion of the stored carbon. These cement plugs are prone to cracking, shrinkage, and detachment from the well interface, potentially resulting in the formation of preferential pathways in which the hydrocarbons can migrate. The consequences are the emission of fugitive CO2, CH4 and H2S into the surrounding environments leading to damage to ecosystems and the atmosphere. This is particularly problematic with the current global push towards net zero carbon. We propose the use of a novel material as an alternative sealant to replace standard cements that should eliminate the formation of these pathways and improve the well's integrity over time. The material, known as Quick Clay, is a naturally occurring, post glacial marine clay of high sensitivity. The clay is from the Quaternary era (2.6 million y.a. –present) and has undergone substantial weathering as a product of glacial retreat and isostatic rebound. The clay is mainly found in northern Russia, Norway, Finland, Sweden, Canada and Alaska and is sometimes referred to as Leda or Champlain clays. The specific conditions in which this clay forms provides it with the unique ability to shift from a rigid solid to a free-flowing fluid near instantaneously, before returning to a relatively strong remoulded state. The project aim is to provide a long-term barrier to limit the emission of remnant hydrocarbons within abandoned wells. In this research work, we investigate the effects of clay density (water/clay ratio) and pore-water chemistry on the mechanical and hydraulic properties of the proposed barrier material. Initial testing indicates that the clay can be pumped at densities similar to that of cement but at much lower viscosities, aiding in the ease of placeability, and preserving its low permeability. Once placed, the clay remains ductile enough to be remoulded and reshaped upon significant deformation, providing a barrier with a self-healing capability. The presentation will show a fundamental characterisation of the quick clay (pH, liquid/plastic limits, mineralogical composition, and particle size), and a parametric study on the pumpability, penetration, compressibility, and shear strength towards a proof of concept for the clay to act as a new sealing element.

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154

SMARTWATER FLOODING: ASSESSMENT OF MOLECULAR STRUCTURES AT OIL/BRINE INTERFACES

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SmartWater, through salinity and ionic strength adjustment, can be a favorable influence on rock wettability and oil recovery. Recent studies revealed information about strong physicochemical interactions of SmartWater with carbonate minerals and crude oil components leading to increased oil production when compared to conventional water injection. To explain this phenomenon, several interaction mechanisms were proposed such as ion exchange, rock dissolution, surface charge changes and many others. Surface charge alteration has been investigated as the most possible hypothesis by several researchers. The previously applied characterization methods have certain limitations to identify the chemical structures at interfaces.

In this paper, advanced Sum Frequency Generation (SFG) spectroscopy, in combination with Zeta PALS, is applied to characterize the chemical structures of molecules and surface charges at oil/brine interfaces. Synthetic brines with different ionic compositions and model oil are used to determine the effects of individual and combined ions on the monolayer structures before and after surface charge alteration. Stearic acid is also mixed with hydrocarbons to mimic carboxylic acids present in the reservoir crude oil. The measurements were conducted with time at broad wave numbers ranging from 1,400 to 3,800 cm-1.

The results obtained from combination of the SFG and zeta PALS methods shed several new insights into understanding not only the chemical structures of monolayers at the interface but also the resulting changes in zeta (ζ) potential as a function of ionic composition. The measured spectra and intensity from SFG are discussed in terms of composition and structure of organic and inorganic components. At the same time, the ζ potential of the model oil droplets in brines was also measured to monitor the surface charges. It was found that the intensity of SmartWater at a certain wave number is higher when compared to conventional injection water and the ζ potential results also showed similar trends to agree with SFG findings. Such consistent results from two different experimental techniques indicate that the interactions at oil/water interfaces are enhanced at lower ionic strengths, which can be considered favorable for oil recovery enhancement.

The uniqueness of this interfacial characterization study is that it provides better understanding of the reaction mechanisms regarding impact of the ionic strength and salinity of injection water due to surface charge alteration at the interfaces. This understanding will be useful for optimizing the chemistry of injection water for improved oil recovery in carbonates.

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Energy Transition Focused Abstracts:

MS17 / 155

Arctic bryophytic cover seen as a porous medium: coupled experimental and numerical thermal properties' assessment

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Thermal regimes of arctic soils are strongly correlated to the presence of perennially frozen soil layers (permafrost). These soils undergo a cyclic annual freeze-thaw phenomenon with the formation of an active layer during summer. A complex patchwork of low vegetation layer consisting of Sphagnum moss, lichen, and peat covers this active layer. Such profiles are found in boreal regions for millions of km².
The latest IPCC reports show that arctic regions are highly vulnerable to climate change.
This vegetation cover proved to be crucial for modelling thermal soil regimes, both at watershed scale [1] and at continental scale [2]. This layer is the main interface between the atmosphere and the geosphere, through which energy and matter fluxes are mainly occurring by evapotranspiration [3]. Assessing morphological, hydraulic and thermal properties of this vegetation layer is thus compulsory to enhance predictive climate change impact models on boreal regions.
However, field measurements are difficult to conduct properly due to the large scale and the poor accessibility of the study area. To do so, some usual porous media study techniques (Representative Elementary Volume study, Pore Network modelling) has been applied in order to quantify morphological properties and hydraulic properties [4]. This first study showed the existence of Representative Elementary Volumes and that the bryophytic cover is highly porous and water conductive.

In the present work, the assumption to consider arctic vegetation cover as a porous medium is extended to thermal properties' assessment. A coupled experimental and numerical approach is set up to cross-validate the results found using both methods.
For this work, 12 dried samples extracted in 2018 at Khanymey Research Station (Siberia) are studied as well as some alive samples extracted from Clarens (Upper-Pyrenees). These samples consist of eight Sphagnum moss samples, two lichen samples and two peat samples.
The experimental setup is based on an enhanced version of the EN 12667 [5] norm for the assessment of thermal conductivity of highly thermal resistive material. Effective thermal conductivity and thermal diffusivity are extracted from thermocouple data and heat flux data coupled with infrared thermography. The values are then averaged to a continuous medium by bisection method.
A two-phase numerical simulation is after conducted on a macroscale tridimensional reconstruction of samples obtained by X-ray tomography.
Samples'thermal conductivity is then fitted to cope with the averaged continuous medium and leads to the cross-validation of the experiments.

The preliminary results show that most of the studied vegetal cover samples are thermally resistive, in-line with field measurements [6]. Infrared thermography shows high heterogeneity in thermal response. Yet, some further work is needed to better understand the linkage between water saturation and hydraulic and thermal properties'variability. Such study allows the generation of

computationally-efficient boundary conditions of this bryophytic layer for large scale climate change impact models.

Participation:

In-Person

References:

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MS08 / **157**

Three-Dimensional Imaging of Density-Driven Convection in Consolidated Rock Samples Using X-Ray CT Scanning

Authors: Anna-Maria Eckel[None]; Ronny Pini[1]

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The determination of realistic rates of CO2 dissolution associated with geological CO2 storage in deep saline aquifers requires an understanding of the mixing process that takes place during the emplacement of CO2 into these formations. The mixing process is triggered by the local density increase in the ambient brine following the CO2 dissolution. As a result, gravitational instabilities occur, and perpendicular elongated finger-like patterns form that are enhancing the mixing between CO2 and water compared to a purely diffusive process. This density-driven mixing process is important because it accelerates the CO2 dissolution into brine and could eventually form a stable stratification in the aquifer, thereby reducing the chances of leakage.

Owing to the difficulty of imaging the time-dependent convective process, experiments so far have largely focused on two-dimensional systems (e.g., Hele-Shaw cells), which inherently limit the lateral spreading of the downwelling plumes. Here, we present the development of an experimental approach to investigate the evolution of the convective mixing process in three-dimensional porous media using X-ray Computed Tomography. To this end, we have considered consolidated rock samples (two sandstones, two carbonates), for which observations have thus far been lacking.
We characterize the rocks based on the different scales of heterogeneities using different measures such as the representative elementary volume (REV), the coordination number and the pore size distribution.
To imitate the dissolution process of CO2 in brine in the rocks under laboratory conditions, a salt is used with a high X-ray attenuation coefficient that dissolves in water and creates a heavier solution than pure water. We observe that the mixing structures, that arise upon dissolution in the consolidated rock samples, differ among those and are strongly impacted by heterogeneities, especially by macro-heterogeneities such as fractures and vuggy pores.
A key advantage of the three-dimensional X-ray CT images is the possibility to monitor and compare the temporal evolution of individual plume structures between the different rock types.
Further, we compute the temporal evolution of the spatial moments of the vertical concentration distribution, including the cumulative dissolved mass, the location of the centre of mass and the spreading length. We find correlations between the scaling of the moments with the heterogeneities of the pore space. This suggests that apart from characteristics of the advective transport (such as permeability and porosity, included in the Rayleigh number), other micro- and macro-structural features are influencing the overall mixing.
These observations provide therefore more representative information towards the investigation of convective mixing in the context of CCS as well as the selection and evaluation of sequestration sites.

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In-Person

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Energy Transition Focused Abstracts:

Poster / 158

Enhanced fluid-fluid chemical reaction kinetics under dynamic multiphase flow

Author: Xueyi Zhang[1]

Co-authors: Zhi Dou [2]; Joaquin Jimenez-Martinez [3]

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Understanding reactive solute transport in natural media is critical for many applications (e.g., groundwater remediation, carbon storage, and enhanced oil recovery). It has already been confirmed that

solute mixing can be significantly enhanced when decreasing the saturation, which ultimately increases effective reactivity. Most studies have been conducted in steady state conditions, i.e., constant flow rate and immobile immiscible phase (e.g., gas or oil) within the pore space. However, in a dynamic multiphase flow system, the motion of the immiscible phase constantly alters the effective flow paths and increases the complexity of the flow field. The impacts of dynamic multiphase flow on reactive solute transport remain an open question. To this end, we build up a quasi-2D porous medium using a 3D printing technique. The new device allows the injection of the reactants together with a steady multiphase flow. We directly evaluate the evolution of a mixing limited reaction by capturing the light emission from an optimized chemiluminescence reaction. Direct numerical simulations are used to infer the velocity field within the liquid phase. In steady state conditions, after an initial increase, the effective reaction rate decreases monotonically. However, while multiphase flow enhances mixing, the effective reaction rate fluctuates in time. Immiscible phase displacements suddenly put two reactants in contact, changing dramatically the local reaction rates in space and time.

Participation:

In-Person

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MS15 / 159

Quantifying pore surface roughness of sedimentary rocks based on SEM images using artificial intelligence techniques

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Co-authors: Mehdi Shabaninejad [2]; Hamed Aghaei [1]; Veerle Cnudde [3]

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Surface roughness of pore space of sedimentary rocks plays an essential role in various processes, e.g., enhanced oil recovery from reservoir rocks [1] and microbially-induced calcite crystal growth [2]. Regarding immiscible fluid flow, the surface roughness affects the local contact angle and hence the relative rock surface tendency to one of the fluids [3]. The roughness impact is much more pronounced for low-conductive porous media where the average diameter of capillaries is small compared to the average surface roughness [4]. In this study, we illustrate an approach to measure the pore surface roughness of sandstone rock by employing extremely high-resolution FESEM images. The procedure adopted in this study was to use a search window over the 2D image data to look for the pore pixels and determine several factors, such as channel size and pixels on the perimeter that were in contact with the rock phase. The speed of the moving window approach was enhanced

by search optimization approaches such as the genetic algorithm, the Monte Carlo method, artificial immune systems, and the particle swarm method [5]. Three common simplified geometries of the sinusoidal curves and squarish and triangular shapes were utilized to determine local roughness values. The information generated in this study included both the extreme surface roughness values and the local pore sizes. Eventually, to unify all these data, we used a neural network to predict surface roughness with respect to microchannel (pore) diameters. The results showed that methods with strong local search such as particle swarm optimization were more effective to find microchannels, while techniques like the Monte Carlo method that has no local search potential were more successful in the search for different roughness values. Our novel methodology for determining pore surface roughness can be used to assess the effects of roughness on phenomena such as fluid flow, surface reaction, and deposition/adsorption inside porous materials.

Participation:

In-Person

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MS06-A / 160

Investigation of factors affecting the performance of surfactant and polymer floods in sandstone cores aided by X-ray CT imaging

Authors: Andrea Rovelli[1]; Ronny Pini[1]

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Traditional oil recovery methods typically extract around 30% of oil within a reservoir; as such, the development and understanding of newer recovery techniques is becoming more instrumental as focus in production shifts away from exploration and into the maximisation of output from already accessible reservoirs. Among these techniques, surfactant/polymer methods have the capability of

increasing recovery up to 70% by both liberating trapped oil, in decreasing the residual oil saturation, and improving the displacement efficiency, in decreasing the mobility ratio. Despite its theoretical efficacy, cost and difficulties with forecasting field scale behaviours are often limiting factors in industrial application. Given the large number, and associated variability between explored cases, of key rock and fluid parameters influencing the displacement process, a traditional workflow firstly involves characterisation tests to determine key fluid properties and corefloods to evaluate the ultimate recovery performance. Within this workflow, the coreflood outlet analysis is critical in allowing for almost all key performance indicators to be inferred; however, given this limited viewpoint, it can be often challenging to decouple, and associate, the observed behaviours in the outlet analysis with the actual behaviour in-situ of the rock cores.
To this aim, direct visualisation of the core flooding phenomena can help elucidate the various contributing factors to the displacement process and help build associated fundamental understanding. Among the available techniques, X-ray computed tomography allows for the visualisation of phase flow, yielding insights into the formation and propagation of the oil bank –characteristic feature of surfactant and polymer floods.

In this work we present results from a series of surfactant-polymer floods performed in Bentheimer cores imaged via X-ray CT where saturation profiles –ranging from one to three dimensional – are extracted. Within these experiments, core aspect ratios and surfactant choice, hence performance, were systematically varied in order to gain appreciation for their respective effects on the fluid phases'flow and oil bank dynamics. Despite similarities in their successful performance by an oil cut and oil recovery viewpoint, direct imaging of the experiments reveals important differences. In examining the internal saturation profiles, we note disparities both in the degree of self-similarity and in the presence of late-stage tailing at the profiles'rear; hinting at differences in both the velocity and the efficacy of the displacement respectively. Through the three-dimensional imaging, other differing effects between experimental cases, such as gravity effects and oil bank dynamics, can also be visualised and quantified. Overall, the length of the core appears to have a strong influence on the 'idealness'of the surfactant and polymer displacement process; despite this, the surfactant choice itself, and its associated performance, can help mask some of the non-idealness –meaning an accurate understanding of the surfactant performance within the core might be limited when examining performance based solely on outlet sampling parameters.

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In-Person

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Poster / 161

Novel laboratory apparatus for understanding microbiology in hydrogen storage in porous media

Authors: Simon Gregory[1]; Jessica Mackie[1]; Megan Barnett[2]

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Controllable but realistic representation of subsurface gas storage scenarios are needed to assess the impacts that microbial processes could have on behaviour of stored gas in hydrogen storage. Current experimental approaches may misrepresent the type and magnitude of microbial activity as they do not consider the limited residual water available as habitats for microorganisms. Understanding microbial processes is necessary as microorganisms could consume and produce gases (including converting hydrogen to corrosive hydrogen sulphide or to methane) or block flow pathways with biomass or precipitates. These processes can only be properly assessed if the gas filled, residual water state can be recreated in the laboratory.
We have developed an experimental set-up that allows us to study microbial processes in both saturated and unsaturated conditions and change between them to represent fluid movement occurring at the fringes of stored gas during storage cycles. The fringes of stored gas have been identified as a potential hotspot for microbial processes.
The apparatus comprises two 1000 ml syringe pumps attached to a core sample held in a pressurised vessel. The system can be operated at pressures of up to 130 -500 Bar (depending on configuration) which is representative of pressures expected during hydrogen storage cycles. The sample can be heated up to at least 90 ℃ to cover the expected activity range of subsurface microorganisms. The system allows the core to be saturated from the base of the sample by flowing a suitable groundwater mimicking the environment in a saline aquifer prior to gas storage. Using the second pump, groundwater can be displaced from pore spaces by injecting hydrogen into the top of the core sample, leaving a residual volume of water more closely replicating the conditions that would occur in a storage reservoir. Continuous logging of flow, pressure and volumes allow the degree of saturation and flow properties to be calculated. Sampling ports allow collection of both gas and water samples, allowing microbial gas consumption and conversion and impact on water chemistry to be monitored.
The apparatus is currently undergoing proof-of-concept testing in which stimulation of methanogens within sandstone cores is being investigated. Although the system most closely resembles hydrogen storage in saline aquifers, it is also relevant to storage in depleted hydrocarbon fields and storage of carbon dioxide.

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162

Real-time Basin-scale Carbon Dioxide Storage Modeling using Fourier Neural Operators

Authors: Gege Wen[1]; Zongyi Li[2]; Qirui Long[1]; Kamyar Azizzadenesheli[3]; Anima Anandkumar[2]; Sally Benson[1]

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Carbon capture and storage (CCS) is an important climate change mitigation technology that captures carbon dioxide (CO2) and permanently stores it in subsurface geological formations. The geological storage of CO2 leads to pressure buildup and gaseous plume migration in the storage formation. Forecasts of these dynamic responses are used to determine CO2 storage capacities and guide important engineering decisions. The modeling of these processes requires multi-phase, multi-physics, and multi-scale simulations, which are very expensive with current numerical approaches.

An especially challenging characteristic of CO2 storage modeling is that it demands both high resolutions and extremely large spatial-temporal domains. The gaseous CO2 plume requires resolutions as fine as one to two meters to provide reliable estimates for the migration. Near-well responses such as pressure buildup and the dry-out effect, i.e., evaporation of formation fluid into the gas phase, also require highly resolved grids around the injection well. Meanwhile, the pressure buildup can travel hundreds of kilometers beyond the CO2 plume and interfere with other injection operations. One approach for reducing the computational costs of numerical simulations is to use non-uniform grids to capture different responses with different resolutions. A popular method known as local grid refinement (LGR) has enabled simulations of real-world three-dimensional (3D) CO2 storage projects, where the fine-grid responses capture the plume migration while the coarser grid responses capture the far-field pressure buildup. However, even with non-uniform grid approaches, these numerical models are still too expensive to be used for important CCS tasks that require probabilistic/repetitive forward stimulation, such as site selection, optimization, and inversion.

In recent years, machine learning approaches are emerging as a promising alternative to numerical simulation for subsurface flow problems. Machine learning models, trained with numerical simulation data, are usually much faster than numerical simulators because inferences are very cheap. However, for CO2 storage problems, the challenge of the multi-scale response has limited developments of machine learning models. Previous studies either focus on 2D problems with a single injection well or 3D problems with very coarse resolutions that fail to capture essential physics.

We present a machine learning framework with an unprecedented capability of high-resolution, full-physics, dynamic 3D CO2 storage modeling. We integrate the FNO machine learning architecture with the LGR modeling approach and present the Nested Fourier Neural Operator (Nested FNO) architecture. Fourier neural operator (FNO) is a type of neural operator that has especially outstanding predictability for flow-related problems by using Fourier transform to learn the solution operator efficiently. This approach vastly reduces the computational cost needed during data collection as well as overcomes the memory constraints in model training. Our prediction resolution exceeds many benchmark CO2 storage simulations run with existing numerical models.

Nested FNO offers dynamic 3D simulations in real time because the prediction speed is 700,000 times faster than the state-of-the-art numerical solver. This prediction speed enables many critical CCS tasks that were prohibitively expensive. The high-quality real-time predictions of Nested FNO can greatly enhance our ability to develop safe and effective CCS projects.

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163

ML-enabled models of ground water transport processes

Author: Mina Karimi[1]

Co-author: Kaushik Bhattacharya [1]

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The transport of water through permeable geological formations couples various phenomena. As the water flows through the permeable medium, water reacts with the medium changing the morphology, mechanical properties, and permeability of the medium; this in turn affects the flow and chemistry. These varied phenomena occur at various length and time scales, which makes the problem extremely difficult. Multiscale modeling approaches have been developed for particular processes to pass the information from one scale to another. However, the actual implementation of this technique is prohibitively expensive. We present a methodology to overcome this challenge by creating a high-fidelity, computationally efficient surrogate of the lower scales behavior that can directly be used at the upper scale to prevent repeatedly solving equations. We particularly focus on the transport of flow through the porous medium in the presence of chemical reactions, where due to the change of internal variables and evolving microstructure, the convection-diffusion equations are complicated. We generate one-time off-line data from the lower scale to train the solution to the partial differential equations over a neural network and obtain a learned surrogate. The surrogate is an inexpensive, approximate solution to the lower-scale problem, which can be used to solve the macroscopic problem without further modeling.

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Energy Transition Focused Abstracts:

164

A Multiphase Energy-based Poromechanics Model for CO2 Injection into Deep Saline Structures

Author: Mina Karimi[1]

Co-authors: Mehrdad Massoudi [2]; Noel Walkington [3]; Matteo Pozzi [3]; Kaushik Dayal [3]

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CO2 sequestration into deep saline structures is an effective and crucial process to control the exponential rise in global CO2 emissions. CO2 injection into deep underground formations requires precise numerical analysis for predicting the stress and pressure distributions in order to prevent leakage, mechanical failure, and induced earthquakes and to analyze wellbore stability. CO2 sequestration problem usually involves multiple fluid phases, and CO2 may experience phase transition, making the simulation extremely challenging. This work presents a multiphase energy-based poromechanics model to simulate the complex behavior of CO2 and predict the pressure distribution during the injection. A variational approach is used to define the governing equations by minimizing the free energy density function of the porous system. A numerical analysis based on the finite element method has been done to analyze the behavior of a multiphase porous system containing CO2 and brine fluid phases. We also investigate the CO2 phase transition in the high-pressure region and the effect of phase transition on pressure and saturation distribution during the injection. This approach can indicate the location of the gas-liquid interface, CO2 phase state, and change of density profile during the injection process.

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Energy Transition Focused Abstracts:

165

Developments of single-phase and multiphase micro-continuum approaches: models to applications

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A diverse range of single-phase and multiphase flow and transport occurs in multiscale porous media. Recently, the micro-continuum Darcy–Brinkmann–Stokes (DBS) approach has been developed to simulate the single-phase and multiphase flow at both the pore and continuum scales via single-field equations. This report reviews the state-of-the-art models and applications, including our latest progress on these issues: (1) A single-phase micro-continuum model was developed to perform an image-based simulation of coke combustion through a multiscale porous medium. The simulation

coupled weakly compressible gas flow, species transport, conjugate heat transfer, heterogeneous coke oxidation kinetics and structural evolution. The accurate numerical results provided a better understanding of coke combustion and can help engineers design sustainable combustion methods; (2) A single-phase micro-continuum model was employed to develop two multiscale workflows to upscale the rock permeability from the millimeter scale to the near centimeter scale. With experimental permeability as the benchmark, this study compared single-scale simulation methods and multiscale workflows to quantify the best permeability analysis method for different rock types, including fractured carbonate, vuggy carbonate, and conglomerate. The acceptable agreement between the experimental and simulated permeabilities for eighteen core plugs improves the confidence in using the developed DRA to predict permeability for complex rocks; (3) A multiphase micro-continuum DBS model to mitigate spurious velocities at the gas-liquid interface and contact-line regions. A series of static and dynamic benchmark cases are investigated to demonstrate that the improved DBS model can simulate capillary-dominated multiphase flows with negligible spurious velocities at capillary numbers as low as 10-4 in both simple and complex geometries. Eventually, some relevant research directions with their challenges are discussed in further research.

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Energy Transition Focused Abstracts:

MS15 / **166**

Physics-informed machine learning application for heterogeneous permeability estimation in 3D sandbox experiments

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Hydrogeological properties are very important to enhance the modeling of physical and chemical processes related to various geoscience and environmental applications such as geologic carbon storage, subsurface energy recovery, and environmental fate and transport. One critical component of subsurface characterization for prediction of flow and reactive transport is how accurately we can estimate heterogenous permeability (and porosity) fields. In this work, we will compare physics-informed machine learning methods such as physics-informed neural network (PINN) and Bayesian PINN to estimate heterogenous permeability fields with spatial and temporal observation data of tracer concentrations in 3D sandbox experiments. Emphasis will be placed on comprehensive state-of-the-art datasets obtained using magnetic imaging resolution approach that provide non-reactive tracer transport over time in well controlled laboratory sandbox experiments. This work will provide outstanding benchmark datasets that can be used for validation of machine/deep learning approaches.
SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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Poster / 167

Semantic segmentation of rock images from multiple imaging methods using deep learning methods

Authors: Robert John Ringer[1]; Hongkyu Yoon[1]

[1] *Sandia National Laboratories*

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Over the past decade non-destructive imaging methods for materials have been increasingly advanced. Two most notable imaging methods include X-ray computed microtomography (μCT) that can image materials at sub-micron scale to millimeter scale resolutions and focused ion beam-scanning electron microscopy (FIB-SEM) that can image at a nano-meter scale. Hence, the segmentation of images obtained from different imaging techniques is a critical step towards quantitatively describing various features of geomaterials over a range of scales. In this work we evaluate various deep learning methods (e.g., U-Net, Attention U-Net, Efficient net, transformer, VGG16, ResNet, and MultiResUnet) to segment both μCT and FIB-SEM images. Four independent datasets including sandstone, carbonate chalks, and shale are evaluated. Each of these datasets is composed of three-dimensional image stacks and corresponding ground truth segmentation labels obtained using various traditional image processing techniques. Our preliminary results indicate that deep learning architectures can successfully be applied to the task of semantic segmentation for individual dataset with frequency weighted accuracy between 94% and 99% (on testing data) and can perform better than manual segmentation to recover the natural morphology of original images. However, performance is significantly deteriorated by ~ 10-30% in accuracy when mixed images from different imaging methods are used as training data. Here, we will demonstrate the improvement of semantic segmentation of multiple rock images from both μCT and FIB-SEM through transfer learning of transformers and other deep learning methods.
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Poster / 169

A Correlation for Dispersion Coefficient in Pipe Flows

Author: Yang Liu[None]

Co-authors: Wenbo Gong ; Moran Wang

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Mixing occurs when two miscible fluids are brought into contact. Dispersion is a homogenized manifestation of the mixing process, which averages velocity and concentration fluctuations that cannot be resolved at the scale of observation. Shear dispersion, the process of solute spreading in pipe flow, originates from the non-uniform velocity profile in a pore cross-section. Taylor dispersion is the asymptotic limit of shear dispersion, i.e., when the pipe is long enough.
In the limit of long times, Taylor [1] derived the advection–dispersion equation for the cross-sectionally averaged concentration with an effective dispersion coefficient. This effective dispersion coefficient is analytically given as a function of Pe, where Pe=UR⁄D_m is the Péclet number expressed in terms of the mean velocity U, tube radius R, and molecular diffusion coefficient D_m. For a tube of finite length, the dispersion exhibits the pre-asymptotic behavior, where the dispersion coefficient, defined by the temporal derivative of the mean square displacement of tracers, increases with flow time and eventually converges to the Taylor dispersion coefficient. There are numerous studies that seek to find the early-time solution for dispersion in straight tubes. However, due to the difficulties of theoretical analysis, most of the studies focused on tubes of circular cross-sections [2]. Since the cross-section of pore structures is highly irregular, it is difficult to upscale these pore-scale studies to the porous media scale.
In this study, we propose a correlation of dispersion coefficient in tubes of different cross-sections. The proposed correlation relates the dispersion coefficient to Pe and flow time. The present study can be easily combined with other simulation methods, such as pore network models, for upscaling the pore-scale shear dispersion to porous media scale.

Participation:

In-Person

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Energy Transition Focused Abstracts:

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Analytical prediction of the relationship between permeability and formation factor accounting for percolation thresholds

Authors: Yannick Nkocko Awountsa[1]; Hardus Diedericks[1]; Francois Smit[1]; Sonia Woudberg[1]

[1] *Stellenbosch University*

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Several authors in the literature have studied the relationship between the formation factor for electrical conductivity and the permeability of different types of reservoir rock by providing stochastic replicas of rock samples and/or performing experimental measurements (e.g., Liang et al. (2000)). The permeability is known to be indirectly proportional to the formation factor and directly proportional to the square of a characteristic length, which can, for instance, be determined from the hydraulic diameter or specific surface area. Walsch and Brace (1984) have determined the hydraulic diameter from the Carman-Kozeny equation which involves an empirical coefficient. Thompson et al. (1987), however, made use of percolation theory to define the characteristic length as the smallest pore size at the percolation threshold. The permeability-formation factor (k-F) relationship has furthermore been extended by, e.g., Revil et al. (2014), by incorporating a percolation threshold porosity, but still containing an empirical exponent. Alternatively, the k-F dependence is expressed as a power-law (in millidarcy), with the coefficient and exponent being empirical parameters. Nkocko Awountsa et al. (2022) have proposed an expression or the formation factor as a function of porosity for isotropic granular porous media in which a percolation threshold porosity is incorporated. This analytical model is based on the Representative Unit Cell model (RUC) model which has served well in the literature. In this study the RUC model will be used to provide an analytical expression for the k-F relationship, which does not involve empirical parameters. The permeability is derived from sound physical principles and related to the formation factor through a geometric factor. The model predictions are validated against experimental data obtained from several authors from the literature for the permeability and formation factor. The data are for actual sandstone rock samples as well as for digitally reconstructed rock samples. Several authors have obtained model predictions for either the k-F relationship, the permeability-porosity relationship or the formation factor-porosity relationship, all within a factor of three from the experimental data. Biella et al. (1983), for instance, have obtained this result for their k-F relationship evaluated against data for artificial clean sand samples of the same characteristic length. Similar results have been obtained by Liang et al. (2000) for their formation factor computed from stochastic replicas evaluated against data of five reservoir rock samples. The average deviation obtained in this study for the model predictions for the k-F relationship compared to the experimental data are also of the same order of magnitude. The advantage of the model used, is that the dimensionless permeability can be evaluated without the need for predetermined curve fitting parameters. The model of Thompson et al. (1987), although also being a theoretical model, requires the measurement of their characteristic length and hence the model cannot be evaluated against other data in the literature for which this dimension is unknown. This study aids to the development and understanding of transport phenomena in the reservoir engineering and petrophysical environments.

Participation:

Online

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Energy Transition Focused Abstracts:

171

Droplet evaporation at the interface of a coupled free flow –porous medium system: Modelling and analysis

Authors: Maziar Veyskarami[1]; Rainer Helmig[1]; Carina Bringedal[None]

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The interface between the free flow and the porous medium in a coupled system has a major influence on the behavior of the whole system. Droplet formation on the interface affect the interaction between the free flow and the porous medium by altering the coupling conditions [1, 2]. Droplet formation and evaporation are of great importance in industrial applications such as water management in fuel cells and cooling systems and even in our daily life where the sweat droplets emerge on our skin . Here, we present the model we recently developed to take the impact of the droplet formation and evaporation on the interface into account. In addition, we used the model to analyze how free flow conditions, such as free flow velocity and relative humidity, and porous medium conditions, such as contact angle and pore temperature, affect the droplet evaporation. In the model, we extended the pore network model developed by [3], which describes the porous medium, to include droplet formation on the interface. Navier-Stokes equations describe the free flow domain. These analyses try to give a better insight about the droplet formation and evaporation.
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MS09 / 173

Direct numerical simulations of turbulent flows over a water saturated porous medium: How two phase pore flow forms roughness at a permeable surface

Author: Johannes Müller[None]

Co-authors: Bernhard Weigand [1]; Hanchuan WU ; Martin Schneider [1]; Rainer Helmig [1]

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Evaporation from a porous medium into a free flow is one of the fundamental processes in environmental systems (e.g. the evaporation of water from soil into the atmosphere [1]). In technical systems self-pumping transpiration cooling can be realized with the help of porous materials where the combination of capillary action and phase change is a promising approach to cool structures due to its high cooling efficiency [2]. The distribution of liquid in the porous material, namely the existence of continuous liquid pathways to the surface of the porous medium influences significantly the evaporation rate [3]. Furthermore, the condition of the turbulent boundary layer in which the vapor is transported away from the surface is of great importance.
Hybrid-dimensional models are successfully used for the efficient modeling of such systems under laminar flow conditions [4]. These models use coupling conditions to ensure the continuity of mass, momentum and energy between the pore network model (PNM) and the free-flow domain. But these coupling conditions comprise unknown parameters (e.g. the slip length) and their validity for turbulent flows is unclear. One possibility to evaluate the validity of coupling conditions and to derive closures for the unknown parameters is to fully resolve the Navier–Stokes equations in the free flow and the pore space.
In this talk results of such pore resolved calculations are presented for a porous medium with different water saturation levels. The focus will be on the momentum balance at the interface. It will be discussed (i) how the rough, permeable surface influences the turbulent boundary layer, (ii) how the fluid distribution will influence the effective roughness and (iii) how the pore wall wettability influences the fluid distribution.
Finally a possible approach for a coupling condition for the momentum balance of a turbulent flow with a porous medium under different saturation levels is presented.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS09 / **174**

A numerical study of CO2-CH4 displacement in shale using Lattice Boltzmann method

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A large portion of shale gas is stored in the kerogen matrix as an adsorbed phase, responsible for the slow production after primary recovery. During CO2 injection, the preferential adsorption of CO2 over CH4 in the shale organic matrix facilitates the desorption of CH4; therefore, gas recovery can be potentially enhanced. In this study, the Navier-Stokes equation and the advection-diffusion equation are coupled in the Lattice Boltzmann method to simulate the CO2-CH4 displacement in two-dimensional dual-porosity porous media. The Langmuir adsorption kinetics is implemented at solid surfaces for mass exchange between the free space and solid matrix. The adsorbed gas is assumed to diffuse within the solid matrix homogeneously. The coupling scheme is validated by comparing the simulation results with the analytical solutions for mass transfer. A convergence study is performed for the lattice resolution and the number of extended layers at the inlet/outlet. The lattice Boltzmann model is robust and efficient in porous media of irregular complex geometries. Preliminary results show that the CO2-CH4 displacement is controlled by the inter-solid and intra-solid mass transfer as well as the mass exchange rate between them. The gas diffusion coefficient, adsorption/desorption rate constants, and pore geometry can affect the concentration and adsorption evolutions of CO2 and CH4.

Participation:

In-Person

References:

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MS11 / 176

Colloidal transport and clogging of a rock-like porous medium: effects of concentration, hydrodynamic stresses and geometry on particle deposition.

Author: Anne-Sophie Esneu[1]

Co-authors: Jalila Boujlel Younsi [1]; Claire Marlière [1]; Lahcen Nabzar [1]; Arnaud Erriguible [2]; Samuel Marre [2]

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Geothermal fluids are often loaded with mineral and organic particles in suspension, various additives, microorganisms, heavy metals, etc. These compounds result in significant problems on the sustainability of production and the maintenance of injectivity in the short term and, in the long term, on the stability and continuity of the resource. As the migration and deposit of fines concern numerous industrial applications, the physics of colloidal particles in porous media has been widely studied. Historically, most of experimental studies were based on macroscopic measurements, mostly with corefloods. Since the media (rocks) are opaque, there is currently very little experimental data describing the mechanisms involved at the pore scale. Lately, interesting results on colloidal deposition and permeability damage have been obtained using microfluidic devices (Bacchin et al., 2014; Delouche et al., 2020, 2022; Dincau et al., 2022; Duchêne et al., 2020; Kim et al., 2022). However, experiments are often conducted on simplified pore-network micromodel or microchannels with or without constrictions, that are not reproducing real porous media. Thus, in this work we focus on micromodels representative of a rock-like porous medium from the intrinsic properties point of view (permeability, porosity, geometry of the pores⋯), to describe the characteristics of permeability damage processes under conditions similar to those of geothermal energy (high flow rates, high permeability ⋯).

The use of microfluidics, which allows direct visualization of the phenomena involved at the pore scale and their quantification through advanced optical methods, was coupled to other important measurements such as pressure.
More particularly, two experimental set-ups have been developed and used, based on different visualization techniques: optical imaging and laser-induced fluorescence (LIF) imaging. Both systems have been designed to integrate the following tools: particle concentration monitoring, pressure drop kinetic, direct visualization of the micromodel in which the fluids are injected. The use of these two technics allows us to access complementary information at various scales. With fluorescence,

we obtain the concentration field that includes the depth of the micromodel, whereas with classical optical imaging we obtain a better resolution of the images and therefore a better understanding of the mechanisms that result from the interaction between hydrodynamics (velocity, pore geometry, ⋯) and DLVO forces (particle-particle and particle-surface).
Indeed, this experimental study allowed to establish links between the velocity field and the characteristics of the deposit; several "types"of deposits related to the geometry of the porous medium have been highlighted. Clogging of pore-throats is a key mechanism for reducing permeability, but pore bodies can also be critical deposition zones under certain conditions and stages of injection. It has been also shown that, as the concentration of the suspension increases, the kinetics of permeability reduction is delayed, and the clogging mechanisms as well as the type of deposit evolve. Finally, at very high concentrations, significant hydrodynamic effects have been observed.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 177

Investigating mass transfer relationships in stereolithography 3D printed electrodes for redox flow batteries

Authors: Maxime van der Heijden[1]; Marit Kroese[1]; Zandrie Borneman[1]; Antoni Forner-Cuenca[1]

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Redox flow batteries are a promising option for large-scale energy storage, but their stringent cost requirements hinder widespread deployment. One option to increase cost competitiveness is by improving the power density of the electrochemical cell by enhancing the performance of the porous electrode microstructure, which determines the available surface area for electrochemical reactions, electrolyte transport, and fluid pressure drop [1]. Conventional porous electrodes are fibrous mats assembled in coherent structures repurposed from fuel cell gas diffusion electrodes [2]. And, while

functional, these materials have not been tailored to sustain the requirements of liquid-phase electrochemistry. Hence, new manufacturing techniques need to be developed affording a higher control over the electrode microstructure and resulting properties. Additive manufacturing, or 3D printing, is an emerging approach to manufacture controlled and deterministic architectures, enabling the tuning of electrochemical performance and hydraulic resistance [3].
In this study, we manufacture model grid structures using stereolithography 3D printing followed by carbonization (Figure 1a) and explore their application in redox flow batteries. We employ microscopy, tomography, spectroscopy, fluid dynamics, and electrochemical diagnostics to investigate the impact of the electrode structure on the fluid and mass transport of ordered lattice structures in non-aqueous redox flow cells. We investigate the influence of the flow field, printing orientation, and pillar geometry on mass transport (Figure 1b). We elucidate correlations between the electrode structure and performance metrics including pressure drop, surface area, and mass transfer correlations. We find that the printing orientation influences the electrode performance through a change in electrode morphology caused by surface roughness and resin spreading, impacting the shrinking direction after carbonization, internal surface area, and therefore the charge transfer, mass transfer, and hydraulic resistances. Moreover, mass transfer rates within the electrode are enhanced by using an interdigitated flow field or by altering the pillar shape to a helical or triangular design, which could improve mixing. Compared to commercial carbon-fiber electrodes, the pressure drop is significantly reduced (Figure 1c) because of the larger pore sizes (~500 µm for the 3D printed electrode vs. 2-100 µm for the Freudenberg H23 paper electrode and 2-300 µm for the ELAT Cloth electrode). Whereas the commercial electrodes feature a superior internal surface area, their area-normalized mass transfer coefficients are lower compared to the printed electrodes (Figure 1d). Going forward, the use of additive manufacturing enabling finer features combined with carbonization at elevated temperatures can be utilized to manufacture multiscale electrodes concurrently providing excellent electrochemical performance and low hydraulic resistance. Combining additive manufacturing with emerging computational topology optimization approaches could enable the bottom-up design of advanced electrode materials for electrochemical devices [4].

Participation:

In-Person

References:

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179

Investigation on water-oil displacement efficiency in heterogeneous porous media based on Voronoi tessellations

Author: Ziwei Liu[1]

Co-authors: Yongfei Yang [2]; Jun Yao [2]

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The pace of research on tight oil exploration and development has been accelerating in recent years. However, the tight reservoir has the characteristics of stronger heterogeneity, more complex pore-throat structure, and smaller pore-throat radius, which hinder their development. Microscopic heterogeneity of pore-throat structure significantly affects the characteristics of oil and water migration and the distribution of microscopic remaining oil. Therefore, research on porous media with strong heterogeneity and complex pore-throat structure has important engineering value. In this work, the water-oil displacement process in heterogeneous porous media was simulated by coupling the Navier-Stokes equation with the phase field method to track the interface between two phases in real time. In the past, the classical spherical grain was often used to study the displacement efficiency of porous media. However, with Voronoi tessellations embedded in porous media as the research object, and randomly subtracting some polygons to form vugs, so as to get closer to the real core structure, it is possible to observe new pore-scale phenomena that are not seen in classical spherical grains. The influence of capillary number (Ca), oil-water viscosity ratio (M) and wettability on displacement efficiency has been investigated. The results demonstrate that at high viscosity ratio and low Ca, the strong heterogeneity caused by vugs makes the dominant channel more unstable, which is the main reason for increasing capillary number does not guarantee higher displacement efficiency under strong heterogeneity. In addition to that, a phenomenon of self-imbibition is observed due to strong heterogeneity, which leads to the coexistence of capillary fingering and viscous fingering at the crossover. Low oil-water viscosity ratio can improve the stability of displacement and make the displacement front more uniform. However, the lower the oil-water viscosity ratio, the higher the displacement efficiency is not. The appropriate oil-water viscosity ratio is the key to enhanced oil recovery. In addition, the displacement efficiency is the highest under the condition of near neutral wetting. Our research shows that for tight reservoirs with poor displacement efficiency due to the heterogeneity of pore-throat structure, it can be considered to change the surface wettability to neutral wetting during production design, and a lower injection rate should be selected to improve oil recovery.

Participation:

Online

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MS09 / 180

Study on Convective Drying of Porous Media –Comparison of Phase Field Simulations with Micro-model Experiments

Authors: Lukas Maier[1]; Sebastian Brosch[2]; John Linkhorst[3]; Matthias Wessling[4]; Ulrich Nieken[1]

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Convective drying of porous media is central to many engineering applications, ranging from spray drying over water management in fuel cells to food drying. To improve these processes, a deep understanding of drying phenomena in porous media is crucial. Therefore, detailed simulation of multiphase flows with phase change is of great importance to investigate the complex processes involved in drying porous media.
In this contribution, we propose a Navier-Stokes Cahn-Hilliard model coupled with balance equations for heat and moisture to simulate the two-phase flow with phase change. The phase distribution of the two fluids air-water is modelled by the Phase Field equation [1].
The focus of this contribution is on the validation and application of the numerical model. While many studies aim to access the phenomena by simulations, here we succeed to compare comprehensively simulations with an experimental methodology based on microfluidic multiphase flow studies in engineered porous media [2]. Comparisons with experiments are rare in literature and usually involve very simple cases. We compare our simulation with convective drying experiments of porous media [3]. Experimentally, the interface propagation was visualized in detail in a structured microfluidic cell made from PDMS. The drying pattern and the drying time in the experiment is very well reproduced by our simulation.

Participation:

In-Person

References:

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MS09 / 181

Starting from the bottom: Coupling a genetic algorithm and a pore network model for porous electrode optimization

Authors: Maxime van der Heijden[1]; Rik van Gorp[1]; Gabor Szendrei[1]; Victor de Haas[1]; Mohammad Amin Sadeghi[2]; Jeffrey Gostick[2]; Antoni Forner-Cuenca[1]

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Porous electrodes are performance- and cost-defining components in modern electrochemical systems as they determine the hydraulic resistance, facilitate mass transport, conduct electrons and heat, and provide surfaces for electrochemical reactions [1]. Thus, electrode engineering is an effective approach to improve cost competitiveness by increasing power density. In convection-enhanced technologies, currently used porous electrodes are fibrous substrates developed for low-temperature fuel cells, but their microstructure and surface chemistry limit the performance of emerging electrochemical systems. Microstructure-informed multiphysics simulations can be leveraged to aid the theoretical design of advanced electrode architectures [2]. However, they have only recently been deployed for the bottom-up design of electrode microstructures [3]. The combination of microstructure-informed multiphysics with evolutionary algorithms could accelerate progress in the optimization of porous electrodes for a given application. In this work, we combine three-dimensional simulations with a genetic algorithm for the bottom-up design of porous electrodes for redox flow batteries.

In the first part of the talk, I will describe a methodology to couple an experimentally validated microstructure-informed, electrolyte-agnostic pore network modeling framework [4] with an evolutionary algorithm [5]. This genetic algorithm is used to optimize electrode microstructures by evolving the structure driven by a fitness function that minimizes pumping power requirements and maximizes electrochemical power output, where the optimization only relies on the electrolyte chemistry and initial electrode and flow field geometries as inputs. The analyzed proof-of-concept employs a flow-through cubic lattice structure with fixed pore positions and shows significant improvement of the fitness function over 1000 generations. The fitness improved by 75% driven by a reduction in the pumping requirements by 73% and an enhanced electrochemical performance of 42%. The evolutionary design resulted in a bimodal pore size distribution containing longitudinal electrolyte flow pathways of large pores and an increased surface area at the membrane-electrode interface.

In the second part, I will discuss our latest progress on the genetic algorithm by implementing integrated flow field geometries, commercial fibrous electrodes as offspring networks, and extended evolutionary freedom during the optimization. Coupling the genetic optimization to the flow field geometry affects the fitness evolution, shifting the balance between electrochemical and hydraulic performance, emphasizing the interaction between flow fields and electrodes. By including additional evolutionary freedom (i.e., by allowing merging and splitting of pores outside fixed coordinates), commercial electrodes can be enhanced by reducing their pumping losses. The presented genetic algorithm offers potential for the predictive design of electrode microstructures tailored for specific electrochemical systems. While applied to flow batteries in this study, this methodology can be leveraged to advance electrode microstructures in other electrochemical systems by adapting the relevant physics.

Participation:

In-Person

References:

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Poster / 184

Wetting and Drying Dynamics in Hierarchically Porous Silicon: An In-Situ X-Ray Microscopy Study

Authors: Stella Gries[1]; Laura Gallardo Domínguez[1]; Mark Busch[1]; Mariia Liseanskaia[1]; Juan Sánchez Calzado[1]; Mathis Boderius[1]; Silja Flenner[2]; Imke Greving[3]; Patrick Huber[4]

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Hierarchical porosities consist of small, often nano-scaled pores as well as large, macroscopic pores to simultaneously achieve large inner surfaces in combination with optimized mass transport. The investigation of the capillary dynamics within optically opaque hierarchically porous membranes necessitates sophisticated microscopy techniques. First hints to unveil the dynamics are obtained from theoretical thoughts and lab-scale experiments, e.g. mass-uptake as a function of time or the mechanical response depending upon wetting and drying in dilatometry. However, these techniques do not spatially resolve on the rising liquid front, which we achieved with transmission X-ray microscopy at DESY's beamline P05. The samples are scanned in radiography (2D) and tomography (3D) to resolve both the static structure and the capillary dynamics. The findings from those experiments can help to tailor hierarchical porous materials for their designated application and to tune the dynamics in wetting and drying depending on the needs.

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In-Person

References:

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Energy Transition Focused Abstracts:

MS16 / 185

Imaging particle transport in thin, porous media using high-speed NMR.

Authors: Olaf Adan[1]; Henk Huinink[2]; ruben nicasy[2]; Bart Erich[3]; Aitor Barquero[4]

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The transport of particles in porous media has received growing attention in the last decades due to environmental concerns in for example the printing industry, the filtration of drinking water and the transport of pollutants in soil. The migration of particles is a complex process which depends on different physicochemical phenomena such as the liquid-particle and particle-media interaction, flow dynamics and the pore morphology. Experimental studies on fast penetration with high resolution are still challenging. In this research, a closer look is taken towards the printing process of water-based inks. One of the most important ingredients which also determine the print quality are latex particles. Therefore, this study aims to follow the transport of latex particles in a variety of water-glycerol mixtures. In this study it is shown that a previous introduced high-speed NMR technique [1] based on the GARField method [2,3] is an ideal tool for studying latex particle penetrations with a temporal resolution of 10 ms and a resolution of 14.5 μm. In order to follow the latex particles within the NMR-setup, magnetic cores are introduced that will modify the signal intensity. The signal intensity is calibrated with respect to the particle concentration, where increasing the particle concentration will decrease the signal intensity. Secondly, penetration experiments with different particle concentrations on porous Nylon membranes with a pore radius of 380 nm were performed. NMR profiles taken at the moment when the fluid reaches the bottom of the membrane are shown in figure 1a. The profiles reveal a splitting of the particle and liquid front which can be seen by the signal increase within the membrane. The positions of the particle front are marked with circles in the same figure. The penetration depth of the particles could also be verified by scanning electron microscopy (SEM) measurement, see figure 1b.
Experiments with varying particle concentrations revealed that increasing the particle concentration will slow down the carrier fluid penetration speed and increase the particle penetration depth. Finally, it will be shown that the method allows to track ink ingredients during capillary uptake by paper sheets.

Participation:

In-Person

References:

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Poster / 186

Aging of liquid foam confined in porous media

Author: Ali Salamé[1]

Co-authors: Vincent LANGLOIS [2]; Olivier PITOIS [3]

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One of the key stages in materials recycling is their crushing into finer elements, i.e. granular material or powder to be sorted and re-used. Insofar as the crushing stage is already very energy-intensive, there is an interest in recycling the crushed elements as directly as possible. In a certain number of cases, simple shaping using a binder, and a possible post-treatment of the peripheral surfaces, would make it possible to produce objects with a useful purpose. Complex liquid foam (liquid foam loaded with a binding component) represents a first-choice low carbon binder precursor to be pushed through the voids offered by a packing made with such grains, to give shape to the whole and to confer significant mechanical strength. This strength is expected to depend on the microstructure of the confined foam, the latter being set by the bubble-to-pore size ratio. Controlling this ratio is not obvious as it is set by the competition between the foam aging rate and the hardening rate of the binder. Indeed, the foam ages, mainly through the so-called coarsening mechanism, which consists in the exchange of gas between the different bubbles, due to their capillary pressure differences, leading to an increase in the average size. When confined, it was shown however that this growth eventually stops when the bubbles have become large enough to be in direct contact with the grains surface.
Here, we show results for the coarsening of liquid foam confined into the porosity of granular packings. During these experiments the liquid fraction is maintained uniform in the system by appropriated rotation of the samples in order to counteract the effects of gravity. Deviations observed with the aging of unconfined foams will be revealed.

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Poster / 187

The impact of multi-scale geological heterogeneities on geothermal reservoir performance

Authors: Kiley Baird[1]; Sebastian Geiger[None]; Florian Doster[None]; Dan Arnold[1]; Carl Jacquemyn[2]; Dmytro Petrovskyy[2]; Jackson Matthew[2]; Gary Hampson[2]; Julio Machado Silva[3]; Sicilia Judice[3]; Fazilatur Rahman[3]; Mario Costa Sousa[3]

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Geological heterogeneities in the subsurface are multiscale in nature, sparsely sampled, and hence inherently uncertain, particularly in geothermal reservoirs where the availability of geophysical and geological data is often limited. Yet, these geological heterogeneities influence the convective and conductive transport of heat in a geothermal reservoir and need to be represented adequately in reservoir models. At which scale the heterogeneities must be captured in static and dynamic reservoir models such that reliable forecasts about safe and sustainable heat production become possible remains an open question.

In this study we use the open-source Rapid Reservoir Modelling (RRM) software to design a series of geological scenarios that contain geological heterogeneities at increasingly more detail. To this end, we consider two geothermal reservoirs where production occurs from a geothermal doublet: one is situated in shallow marine deposits and one in deepwater slope channels. The multiscale geological heterogeneities that characterise these reservoirs are represented through a hierarchy of surfaces that represent stratigraphy, facies, and diagenetic bodies. A key advantage of RRM compared to more traditional modelling approaches is that multiscale reservoir models can be constructed in both, a geologically consistent and time effective way, and feedback on the essential static and dynamic reservoir properties is obtained while building the reservoir models.

Using the flow diagnostics capabilities in RRM, we conduct a first screening of the breakthrough times between injection and production well for different well locations, before commencing more detailed and time-consuming full-physics simulations using a commercial geothermal reservoir simulator. These simulations clearly show that forecasts about reservoir performance and heat production become more variable as more geological details are considered: the small-scale (~1m) heterogeneities have significant impact on reservoir connectivity and lead to significantly lower estimates in energy capacity.

Our work demonstrates that it is crucial to design geothermal reservoir models that represent the geometry and connectivity of reservoir heterogeneities in a geologically consistent way to obtain more reliable estimates about reservoir performance and heat production.

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MS08 / **188**

Topological Control on Flow and Transport in Unsaturated Porous Media from Temporally Resolved 3D X-ray Computed Micro-tomography

Authors: Andrés Velásquez-Parra[1]; Michele Griffa[2]; Rolf Kaufmann[2]; Federica Marone[3]; Joaquin Jimenez-Martinez[4]

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The unsaturated zone, including soil and vadose zone, controls the exchange of water, heat, and chemical substances between the soil surface and aquifers. It also hosts several processes involved in the transfer of nutrients, playing a key role in the availability of life-sustaining resources. Anthropogenic actions, such as agriculture, urban waste management, and industrial activities, add substances to the soil that might compromise the quality of fresh groundwater resources. Being able to predict the fate of such substances in the subsurface through an assessment of flow and transport processes is essential for mitigating their negative effects and for designing more effective remediation measures. We analyze flow and transport processes in unsaturated media at pore-scale using high spatio-temporal resolution X-ray computed micro-tomography (synchrotron). 3D transport experiments through a synthetic sand-like porous medium using a contrast solution were performed at different saturation degrees. Experimental data allowed the reconstruction of the plume' s advancing front and the tracking of its deformation over time, i.e., variation in the surface area of the 50% concentration plane. Results indicate an enhancement of the solute front deformation at lower saturation degrees and at larger flow rates, showcasing the role of the system's heterogeneity in shaping solute dispersion. This is explained by a better connectivity of the system at lower saturation degrees, expressed through more negative Euler characteristic values, which highlights the better performance of the system at connecting initially separated parcels of fluid through the formation of preferential paths and a larger number of stagnation zones. To also link the observed solute front deformation rates with the hydrodynamics in the pore space, the average helicity density in the pore space was computed. Lower saturation degrees resulted in a larger helicity density, indicating a more heterogeneous flow field characterized by larger tortuosity and more complex streamlines, which explains the observed stronger solute front deformation at lower saturation degrees. Implications of these results on transport were assessed via estimation of the Okubo-Weiss parameter, which indicated a stronger control of both shearing and vorticity on solute plume deformation at lower saturation, potentially hinting at an enhancement of mixing rates. These findings represent a major step towards understanding the control of saturation on the hydrodynamic landscape within the pore space and on the deformation rate of solute plumes and fronts, both essential to understand mixing dynamics in unsaturated porous media.

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MS22 / 189

An Efficient Method to Compute Capillary Pressure Functions and Relative Permeability Curves in Dual Porosity Systems Arising in LCM Processes

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Liquid Composite Molding (LCM) is a manufacturing process of composite materials. In this talk, we consider an LCM process in which a textile stack that is at the beginning filled with air is infiltrated with a thermoset polymer resin. The textile stack consists of multiple layers of fiber mats. The fiber mats are made of woven rovings and the rovings themselves consist of hundreds of filaments. The injection process can be modeled as a two-phase flow. A simulation of a two-phase flow in a textile stack with sizes that are realistic for industrial purposes is not feasible on a fully resolved geometry. Because to model the tinny pores between filaments of a roving a very fine discretization is needed.

Alternatively, we consider this as a multiscale problem. In our setup, we distinguish three different length scales. The macroscale is the complete textile component. The mesoscale consists of a section of a few fiber mats stacked on each other and the microscale is a section of a single roving. Now we can use an effective model on the macroscale e.g., the two-phase Darcy model. This model can at least approximate the overall flow field of the infiltration process. To set up this effective model on the macroscale, some effective parameters are needed from the mesoscale. The quality of the macroscale simulation depends on how realistic these parameters are. In the case of the two-phase Darcy model, we need the capillary pressure function, the absolute permeability, and relative permeability curves.

In this talk, a method is presented with which it is possible to approximate these effective parameters on the mesoscale by simulations that treat the rovings as a continuous porous material. This porous material is represented by a microscale geometry. The advantage of this is that the filaments do not need to be modeled in the mesoscale geometry. Then it is possible to use a coarser discretization of the mesoscale geometry without losing much accuracy. Two-phase flow simulations and computations of effective parameters on the mesoscale are not straightforward. Because the geometry consists of the rovings that are given by a porous medium and free-flow regions between the rovings. Among other things, we use GeoDict implementations of pore morphology methods and Stokes or Stokes-Brinkman solvers during the computation. The method is not only applicable to the presented LCM process but also to other dual porosity systems. In the first part of the talk, we present the method. After this it is verified on simpler dual porosity examples and in the end, it is applied to the LCM-process example.

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MS06-A / 190

Model of water drop infiltration in porous media with amphiphilic matter

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Under the current climate change, assessing water transfer and infiltration in soil, considered as complex porous medium, is a crucial point for estimating consequences of either heavy rain on runoff or of drought on plant water uptake. In both cases, variations in soil wettability due to amphiphilic materials is an overlooked point, but can greatly affect the infiltration and water transfer, such as water repellency in soil **[Doerr2000,Orfánus2021,Bens2007]**.

A macroscopic model of the infiltration of a water drop into a porous medium is developed and applied to a soil containing amphiphilic molecules such as Exopolysaccharides (EPS) found in soil near plant roots **[Bérard2020]**. These molecules present a hydrophobic or hydrophilic property depending on the water content in soil. Experiments found in literature **[Liu2012,Hapgood2002]** or performed in our laboratory show two main behaviors :

i) When the soil is sufficiently moist, imbibition is immediate and rapid as in hydrophilic soils.

ii) In contrast, for a dry soil, the drop does not infiltrate immediately and the subsequent imbibition is slower and depending on the soil hydrophobicity, the drop may never infiltrate.

Models based on Richards Equation **[Richards1931]** in the soil and its variants **[Beljadid2020,Landl2021]** can only reproduce the rapid infiltration of regime i). We propose here to derive new equations describing the hydrophilic and hydrophobic interactions both in the soil and on the soil surface in contact with the water drop to describe all water infiltration regimes. In place of a contact angle to characterize the wettability of the soil surface, we introduce a free energy term which includes attractive and repulsive interactions, derived from the modeling of drop dynamics on a substrate **[Thiele2018]** and include the dependence of the surface wettability on the water saturation in the porous matrix **[Doerr2000]**. Concerning the soil, we recently developed a water-dependent hydrophobicity model **[Beltrame2022]** which has been extended to the case of amphiphilic molecules. In order to reproduce to interactions between water at soil surface and in the soil volume, and to be consistent with thermodynamic principles, we show that it is necessary to add a term inside the porous matrix that depends on both the saturation and the film height at the surface. The resulting equation system is a fourth order PDE system similar to the lubrication model with wettability. To our knowledge, it is the first time that wettability, both in the soil and on the soil surface, is accounted for to represent water infiltration. The numerical simulation of developed coupled equations is in agreement with the experiments of the infiltration of a drop on a thin layer of sand containing EPS. We retrieve the dependence of the Water Drop Penetration Time (WDPT) test with the concentration of amphiphilic molecules and soil moisture.
Moreover, we are able to reproduce the two regimes of the infiltration dynamics: instantaneous infiltration and progressive and slow infiltration depending on the initial water saturation of the soil.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS10 / 191

Using 4D-Imaging to describe the impact of the microstructure on sublimation front patterns

Author: Sebastian Gruber[1]

Co-authors: Maximilian Thomik [2]; Frederik Coppens [3]; Nicole Vorhauer-Huget [4]; Evangelos Tsotsas ; Petra Foerst [1]

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Freeze-drying is a gentle drying technique for high value products such as pharmaceuticals. The process can mainly be separated in three steps. (1) The freezing step, here the actual microstructure of the final product can be formed. (2) The primary drying removes the ice out of the product by sublimation. (3) The secondary drying is used to remove the bound water inside the matrix by desorption to get a stable product. While freeze-drying is still a very time and energy consuming process, it is still the aim to accelerate the process [1]. Here one important factor is the microstructure of the product [2]. In literature often the influence of the pore size is described and stated that bigger pores lead to a faster drying because of the lower mass transport resistance. However, other structural parameters such as pore shape and orientation are neglected. Recently we could demonstrate the impact of pore shape and orientation on the movement of the sublimation front in 2D [3]. In this work, we will present a more detailed study on the impact of the microstructure on drying kinetics by using in-situ freeze-drying experiments. For that freeze-drying experiments were conducted with a custom made freeze-drying stage in the 4D tomography system DynaTom. Here, continuous tomography scans were conducted during the freeze-drying experiments to observe the movement of the sublimation front in 3D. At the end of each experiment a high resolution scan of the final microstructure was made. To generate different microstructures, different freezing protocols were used (different solid concentrations and annealing treatment). The experiments are conducted at -15℃ shelf temperature and the chamber pressure is 10 Pa. By the use of an inhouse MATLAB and python script the microstructure in terms of pore size, shape and orientation as well as the movement of the sublimation front are analyzed. It can be demonstrated that depending on the pore shape, either pore size or orientation can be the more dominating factor.

Participation:

In-Person

References:

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Poster / 192

Quantifying the Partial Reversibility of Dispersion in Push-Pull Experiments by Means of Second Central Spatial Moments

Authors: Marie-Madeleine Stettler[1]; Marco Dentz[2]; Olaf Cirpka[1]

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Solute dispersion in heterogeneous porous media is classically parameterized by Fickian-type macrodispersion concepts, matching the rate of change of second central spatial moments. As diffusion is an irreversible process, the second central moments computed by a Fickian macrodispersion model can only increase –also upon flow reversal. By contrast, if solute transport was strictly advective, the second central moments would increase due to heterogeneity in forward motion, and symmetrically shrink upon flow reversal until the plume shape of the initial distribution has been recovered. The interplay between advective spreading and diffusive mixing makes solute dispersion partially reversible. We investigate this behavior for uniform-in-the mean forward and backward motion, considering both the ensemble averaged second central moments of individual plumes that start as points (effective moments) and the second central moments of the ensemble averaged concentration (ensemble moments). The ensemble moments include the uncertainty of the plume's center of gravity, so that effective moments are considered to be more representative for the mixing behavior of single solute plumes. Our analysis includes new analytical results based on stochastic perturbation theory, and particle-tracking random-walk simulations in periodic domains. We investigate (i) how hydraulic medium properties and transport parameters influence the partial reversibility of the effective and ensemble moments, (ii) over which time scales they shrink upon flow reversal, and (iii) how long it takes until the asymptotic dispersion coefficients are practically reached. The perturbation theory results agree well with the random-walk simulations for cases of low log-conductivity variance. We find that parameter changes favoring mixing (increasing variance of the log-K field, increasing anisotropy of the field, decreasing Péclet number, increasing reversal time) lead to a decrease in reversibility. As long as the advective memory dominates, both ensemble and effective moments undergo a finite phase of shrinking upon flow reversal. Before the original starting point has been reached, this is followed by an increase in second central moments once diffusion has made the solute particles forget their exact trajectories of the forward motion. The shrinking phase is shorter and less pronounced for effective moments because at early times, the effective plumes are smaller and sample less variability of the velocity field. Thus, effective moments are less reversible than ensemble moments, and more suited for mixing parameterization, although they are no measure for pure mixing either. In backward motion, even after the moments begin to increase again, the influence of advective memory persists over hundreds of travelled correlation lengths, which implies that it is impossible to run practical applications long enough for the plume to escape the influence of the change in mean flow direction. Overall, our results shed light on the interpretation of dispersion coefficients derived from breakthrough curves in push-pull tests, which, different to intuition, are not measures for pure solute mixing but account for both the mixing contribution to dispersion, as well as for advective solute spreading.

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MS10 / **193**

Development of a tridimensional characterization methodology

for hierarchical materials: application to the nuclear effluent decontamination in fixed-bed processes.

Author: Samuel VANNIER[1]

Co-authors: Agnès GRANDJEAN [1]; Alban GOSSARD [1]; Thomas DAVID [1]; Vanessa PROUST [1]

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Hierarchically structured materials consist in multiphase (crystalline-amorphous) materials also presenting a multiscale porosity. Such materials are widely used for the decontamination of liquid effluents in fixed-bed processes. Indeed, charge-compensating ions in their structure allow them to perform a selective cationic exchange. Their decontamination efficiencies are finely determined using static and dynamic experiments [1]. However, no precise link between their decontamination performances in fixed-bed processes and their multi-scale microstructure has been identified yet. In this way, this project aims to develop reproducible methods and protocols to finely analyze the tridimensional microstructure of hierarchical materials at different scales and correlate these quantitative data to the decontamination properties (thermodynamics, kinetics and hydrodynamic).

For that purpose, the development of efficient characterization methodologies involves the use of different cutting-edge techniques. On the one hand, the way to follow and analyze precisely the various scales of porosity and the localization of the different phases of the materials was identified. On the other hand, the use of numerical methods is necessary to process and combine data to extract key parameters describing the microstructural architecture of these hierarchical materials as finely as possible.

These developments are performed on model materials with adjustable properties. Notably, zeolite powder hosting selective active sites for Cesium has been embedded in a multiporous geopolymer matrix [2]. Techniques such as electron microscopy (2D), electron microscopy with focused ion beam (3D) and X-ray tomography (3D) are used. Image segmentation is performed thanks to advanced numerical methods involving machine learning, which enhance the efficiency and the precision of the process. Various image processing softwares provide numerical values of different morphological parameters impacting the decontamination efficiency like the geometry and tortuosity of the porous network or the localization and accessibility of "active"sites for the decontamination. Correlative data processing will consist in improving data from one imaging technique thanks to results from another. This allows to better investigate the various scales of porosity and their impacts upon the decontamination properties of these hierarchical materials.

Participation:

In-Person

References:

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MS05 / **194**

Meter-scale MICP improvement of medium graded very gravelly sands: lab measurement, transport modeling, mechanical and microstructural analysis

Authors: Guijie Sang[1]; Rebecca Lunn[2]; Grainne El Mountassir[2]; James Minto[2]

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Microbially induced carbonate precipitation (MICP) is a promising biogrouting method for ground improvement and leakage remediation. Most studies to date have focused on MICP treatment of uniform clean sands, with few studies having been conducted at large-scale on well-graded soils more representative of in situ deposits. This study presents a laboratory meter-scale MICP test on medium-graded very gravelly sands consisting of 3.9% fines (< 63 μm) from field. The MICP treatment was conducted in a radial flow cell (diameter: ~1m; thickness: ~0.15 m) with an injection well located at the center and a constant hydraulic head at the outer boundary to replicate field conditions. Aqueous chemistry of the effluent samples at the middle of the central injection well and the outer boundary was continuously monitored, and transport of tracer and bacteria breakthrough in the radial flow cell and in separate 1-dimensional columns was modeled and simulated for a better understanding of the MICP process. The MICP-treated soil was subjected to a series of hydro-mechanical tests and microstructural analysis. Transport modeling and effluent sampling monitoring of the electrical conductivity and pH show that there was an overall good delivery and reaction of the bacteria and chemicals in the radial flow cell, but there also existed preferential flow paths due to soil heterogeneity and fines migration, which caused significant variations in permeability. Interestingly, compared to previous studies, the biocemented core samples with well-graded angular particles in this study had higher strengths (2.6-7.4 MPa) for a given calcite content (9.2-15.1%) than those in comparable studies treating uniform soils. This is likely due to a higher density of particle contacts as a result of both increased particle angularity (as suggested by backscattered electron imaging and X-ray imaging analyses) and higher packing efficiency in the medium-graded very gravelly sand. Consolidated-drained triaxial compression tests on two samples near the injection well showed a peak deviatoric strength of ~5 MPa under an effective confining stress of 500 kPa and a clear shear band was observed upon failure. To summarize, we have successfully achieved an overall good biocementation in the radial flow cell, despite the great soil heterogeneity. The study also suggests that migration of fines and the subsequent formation of preferential flow paths may be a challenge for producing uniform biocementation in field applications of MICP.

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MS05 / **195**

In situ imaging of bacteria transport and attachment in geologic materials using positron emission tomography

Authors: Christopher Zahasky[1]; Vy Le[1]

[1] *University of Wisconsin-Madison*

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Contamination of groundwater by *Escherichia coli* (*E. coli*) bacteria has been a persistent and growing risk to globally strained groundwater resources. Prevention, mitigation, and regulation of contaminants requires a fundamental understanding of the mechanisms of transport and attachment of *E. coli* in complex geological materials under hydrogeologic conditions. This work demonstrates the first experimental quantification of dynamic bacteria transport and attachment distributions in geologic materials using 3D medical imaging. The approach relies on radiolabeling *E. coli* bacteria with positron-emitting radioisotopes and then using positron emission tomography (PET) to monitor bacterial distribution and transport in heterogeneous sand packed column experiments. The results of this study indicate that bacteria attachment coefficient distributions are described by gamma probability density functions. As expected, these functions shift to higher attachment coefficients with decreasing grain size and decreased sediment sorting. Results from these radiolabeling and imaging techniques provide a transformational approach to directly measure and understand dynamic bacteria attachment and detachment behavior in realistic geologic systems.

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Poster / 196

Impact of Relative Permeability Hysteresis on Underground Hydrogen Storage

Authors: Diya Sunil Kumbhat[1]; Anozie Ebigbo[2]

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The relative permeabilities of multiphase fluid systems depend on saturation history as has been shown by experimental, numerical, and field studies. Such hysteresis is especially relevant in underground hydrogen storage (UHS). UHS projects involve temporary storage of hydrogen in the porous subsurface on a seasonal timescale. The injection and production of hydrogen over the span of several seasons necessitates accurate description of saturation history in the reservoir to estimate the overall efficiency of the storage operations and losses due to trapping.

Here, we concentrate on hydrogen injection and production into a heterogeneous semi-synthetic benchmark model of a saline aquifer [1] using TOUGH 3 [2]. We conduct reservoir simulations of UHS accounting for experimental hydrogen-water relative permeabilities from literature [3] which show obvious hysteretic behaviour. The goal is to elucidate the effect of inclusion of hysteretic vs non-hysteretic relative permeability-saturation constitutive relations for multiple storage cycles of UHS. Key markers such as quantity of hydrogen extracted in each cycle and evolution of gas-saturation distribution in the reservoir illustrate the importance of accurately accounting for hysteresis in the simulation of UHS.

Participation:

In-Person

References:

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Poster / 197

Colloid transport inside slow sand filters: A multi scale study

Author: Mandana Samari-Kermani[1]

Co-authors: Amir Raoof [1]; Jack Schijven [1]

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Slow Sand Filters are the last step of producing drinking water in the Netherlands which play a crucial role in removing microorganisms. A biolayer formed on top few centimeters of the sand, called Schmutzdecke, plays an effective role in colloid removal. A multi scale study is performed to investigate removal efficiency of this layer and attachment mechanisms inside these filters. Pilot plant/ column experiments are done at the meter/centimeter scale to study the effect of different operating conditions such as grain size and flow velocity. These experiments are done by seeding Escherichia coli WR1 as a model bacteria into the filters. At the micro scale, microfluidics are used to directly observe colloid-biofilm interactions, biofilm growth and colloid transport inside the porous media. Result shows that biofilm growth can clog the throats, make preferential flow paths, and decrease filters conductivity, while it can increase removal efficiency.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS05 / **198**

Assessing the strength of biomineral strategies for concrete repairs.

Authors: Athanasios Karampourniotis[1]; Gloria Castro[2]; Rebecca Lunn[3]; Enrico Tubaldi[4]; Grainne El Mountassir[4]

[1] *PhD student, Civil and Environmental Engineering, University of Strathclyde*

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[3] *Professor, Civil and Environmental Engineering, University of Strathclyde*

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Worldwide production of concrete is estimated to be responsible for approximately 8.6% of all CO2 emissions originating from human activity [Miller et al., 2016]. Many countries, including the UK, now have ambitious targets to achieve net zero greenhouse gas emissions. To achieve these targets, the construction industry needs to transform its use of materials and approaches to asset management, with a shift towards extending the lifespan of existing structures, rather than constructing new ones.

Microbially Induced Carbonate Precipitation (MICP) is a novel engineered process in which ureolytically active bacteria trigger the catalysis of urea, resulting in the formation of calcium carbonate crystals. MICP shows promise for a wide range of engineering applications including rock fracture grouting, soil strengthening and for stone and concrete repair.

The aim of this research is to develop a mesoscale Finite Elements Model (FEM) to predict the mechanical behaviour of MICP-treated concrete. In order to calibrate the FEM model, MICP treatment and tensile strength tests were conducted on concrete cores.

Seven cylindrical concrete specimens were drilled from a caisson acquired from docks in Devonport, England. Subsequently, the cores were artificially cut along their vertical length creating a single fracture within each core. A variety of filling scenarios were investigated: (i) open fracture with glass bead spacers (500μm in diameter) only present at corners, (ii) patches of glass beads within the centre of the fracture, (iii) fully packed with glass beads, (iv) fully packed with silica sand grains, and (v) fully packed with carbonate sands.

Cores were subjected to multiple treatments of MICP. Each treatment included the injection of *Sporosarcina Pasteurii* (highly ureolytically active bacteria) followed by injection of a cementing solution consisting of calcium chloride and urea. Core permeability was monitored after each treatment

cycle. Treatment was stopped once a 2-order of magnitude reduction in permeability was observed. After treatment, the cores were subjected to X-ray Computed Tomography (XCT) scanning and image analysis was conducted to evaluate the amount and spatial distribution of contact points created by calcium carbonate precipitation bridging across fracture surfaces. Following XCT imaging, the cores were loaded under Brazilian test conditions to evaluate tensile strength. After failure, the patterns of calcium carbonate precipitation on the surfaces of the fracture were inspected, validating the results derived from image analysis.

The experimental results show that the mechanical strength of the MICP-treated cores is governed by the amount of calcium carbonate precipitation which bridges across from one fracture surface to the other. A FE model simulating tensile loading has been developed which can be used to predict the mechanical behaviour of MICP-treated concrete as well as to better understand the influence of MICP treatment strategies on mechanical strength recovery.

Participation:

In-Person

References:

SabbieAMiller, Arpad Horvath, Paulo J M Monteiro. Readily implementable techniques can cut annual CO2 emissions
from the production of concrete by over 20%. Environmental Research Letters 2016;11:074029
doi:10.1088/1748-9326/11/7/074029

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Energy Transition Focused Abstracts:

Poster / 199

Expression of Eshelby tensor from fabric tensor

Author: Young June Yoon[1]

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The mechanical properties of highly porous materials are expressed by fabric tensors. But the structure of highly porous materials is complicated if it is not arranged periodically. In micro-mechanical schemes or homogenization, the Eshelby tensor is widely used to estimate porous materials' mechanical properties. However, the relationship between these two tensors is not known. The result will be given by the equation, but some experiments are required to obtain numerical results.

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Energy Transition Focused Abstracts:

200

Automated Symbolic Upscaling: Model Generation for Extended Applicability Regimes

Author: Kyle Pietrzyk[1]

Co-author: Ilenia Battiato [1]

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In complex multi-scale system analyses involving porous media, coarse-grained models are used to significantly increase computational efficiency and accurately model physical processes across multiple scales. Such models can be systematically generated through rigorous *upscaling* techniques, which provide *a priori* error estimates and conditions under which models are valid (i.e., *applicability conditions*). However, such techniques are often limited to weakly reactive regimes, where resulting upscaled equations only differ from their corresponding pore-scale equations by effective dispersion coefficients and additional reaction terms. This makes it difficult to justify the long implementation times and analytical intractability endured during upscaling techniques, as more *ad hoc* approaches can quickly generate similar models, but with less accuracy and generality. To reduce implementation times and methodically handle analytical intractability while upscaling complex multi-physical, multiscale processes in porous media, we developed Symbolica, a symbolic upscaling framework for accelerated and automated model development. Here, we present a novel strategy for generalized closure problem formulation that enables upscaled model generation with less restrictive applicability conditions, and encode it in Symbolica. In the moderately reactive regime, nontrivial terms are found in the upscaled models, such as effective advection terms that are nonlinear and independent of the fluid velocity, and emergent terms that appear in multi-component reactive systems. Ultimately, the results demonstrate that our automated upscaling framework, Symbolica, is capable of accurately analyzing systems not previously studied in literature, making it relevant and advantageous in both academic and application-based settings.

Participation:

Online

References:

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- K. Pietrzyk and I. Battiato. “Automated symbolic upscaling: model generation for extended applicability regimes, part 2”, (Submitted to Water Resources Research)
- K. Pietrzyk, S. Korneev, M. Behandish, and I. Battiato. “Upscaling and automation: pushing the boundaries of multiscale modeling through symbolic computing”, Transport Porous Med., 140, 313-349, 2021.

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Energy Transition Focused Abstracts:

MS01 / 201

On the conceptual role of permeability contrasts within sandstone utilised for underground hydrogen storage

Authors: Doug Smith[1]; Andreas Busch[2]; Dan Arnold[2]

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Numerical modelling with commercial software (CMG) was used to analyse of the effect of contrasting permeabilities on fluid flow and hydrogen plume development in subsurface, porous media employed in underground hydrogen storage. Increasing heterogeneities were introduced to reservoir-scale simulations, based upon the Navajo sandstone, Utah in an aquifer-supported system. Initial investigations into the effects of well placement on reservoir pressure, cumulative hydrogen and water production in a homogeneous and heterogeneous model were used as baseline simulations to benchmark the performance of scenarios containing further permeability contrasts.

The results show, in terms of well placement, that production well placement at the top of the reservoir is the most important factor to maximise hydrogen production, due to the buoyancy of hydrogen. The relationship between permeability and viscosity in Darcy's equation of flow provides a rudimentary guide to the behaviour of hydrogen in relation to contrasting permeabilities. However, reservoir heterogeneities affect fluid pathways, linking the effects of previous permeabilities, creating compartments and impacting upon the flow of other fluids. These characteristics, coupled with hysteretic effects, affect local pressure gradients, the other variable in Darcy's equation, and determine the hydrogen migration. As a result, forecasts of plume development and reservoir performance need to consider the whole system.

Participation:

In-Person

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Poster / 202

Rayleigh-Bénard instability in heterogeneous porous media

Authors: Rima Benhammadi[1]; Juan José Hidalgo[1]; Marco Dentz[1]

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Convective mixing is present in a large assortment of natural and industrial processes, such as in carbon capture and sequestration, where it ensures a safer storage of carbon dioxide, seawater intrusion, high-level radioactive waste disposal sites and geothermal energy production. In this work, we study the effect of the heterogeneity on the behavior of convective mixing since most of the works that have been conducted so far did not take heterogeneity into consideration.

To do so, we consider the Horton-Rogers-Lapwood problem where convection is triggered by a Rayleigh-Bénard instability. Heterogeneity is represented by 2-D multi-Gaussian log-Normally distributed anisotropic permeability fields. We perform a parametric study in which we explore the effect of the variation of the Rayleigh number (Ra), the variance and the correlation length of the permeability field on the fingering patterns, mixing and dissolution fluxes. Mixing is characterized by the scalar dissipation rate and the boundary fluxes. The mixing state is evaluated through the probability density function of the concentration and the intensity of segregation. We show the difference in behavior between the dissolution fluxes and the mixing state both for the case of homogeneous and heterogeneous porous media. We observe that convective mixing is enhanced in the case of heterogeneous porous media compared to the homogeneous counterparts.
An increase of Ra causes a more rapid homogenization of the system especially for the heterogeneous case. For permeability fields with a small correlation length, the effect of the heterogeneity is substantial only for a variance higher than 2. However, for a larger correlation length, this effect is more pronounced and the fingering patterns are no longer smooth but dispersive.

Based on these observations, an upscaling of the model based on the effective longitudinal and transverse permeability and the dispersion coefficient is performed.

Key words: convective mixing, Rayleigh-Bénard instability, heterogeneity, scalar dissipation rate, dissolution fluxes.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

203

Impacts of microbial biodegradation and biodiversity on petroleum engineering environment

Author: Turan Mutallimov[None]

Corresponding Author: t.mutallimov.22@abdn.ac.uk

The oil and Gas industry has had an enormous impact on the environment, throughout its exploration, production transportation and post-decommission. There is a growing demand to understand the microbial activities as a result of hydrocarbon spillage and this is a particular case for profound impacts on the increasingly decommissioning activity on biodiversity in the seabed and biodegradation in the subsurface such that it has been estimated to ramp up even further over the next decades. The microbial activity on altering the wettability of reservoir rock surface which has a positive impact on EOR has been researched a lot, but its other impact on the environment is entirely a gap.

This project will be focusing on investigating the comprehensive microbial process involved in biodegradation on petroleum production sites and its relevant environmental impact including the microbial biodiversity in the seabed. However, the fact that there are no scientific data or studies available is particularly striking. In this respect, this proposal concerns the impact on microbial populations around the decommissioning platforms using contemporary molecular biology methods because microorganisms are very sensitive to environmental changes. Furthermore, microorganisms are in the subsurface and subtle changes in their population hugely affect other living organisms that are dependent on microorganisms. Therefore, modelling the microbial populations around the oil production field can be used as a prediction of the environmental impacts.

The selection of hydrocarbon degraders in response to oil deposition produced changes in microbial succession. This indicates a quick response of bacterial communities to deep-sea sediment pollution, sped up by dispersant and could be used in oil pollution monitoring equipment. Shallow-sediment consortia had a higher degradation potential than deep-sea consortia, which shows how in situ circumstances affect community structure and repair potential. Highly contaminated river sediments were already adapted to HCs because, after HC addition, their diversity and community structure remained unaltered. In contrast, the addition of HC radically changed the communities of pristine sediment by choosing HC-degraders. These results underline how crucial it is to comprehend how communities are put together and can help in predicting how microbes will react to oil spills. In this work, existing solutions were reanalyzed and new possibilities were explored.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

Poster / 204

The effects of a variable interface permeability on a one-domain VANS model

Author: Bruno Dias[1]

Co-authors: Jeremie B. E. Meurisse [2]; Nagi N. Mansour [2]

[1] *Oak Ridge Associated Universities at NASA Ames Research Center*

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Space exploration has aimed to visit other planets and sample cosmic bodies within our solar system in the past decades. As these ambitions increase, new technologies and the development of lightweight porous materials are needed to design spacecraft Thermal Protection Systems (TPS) that endure the harsh environment of hypersonic atmospheric entry and ensure the safety of the payload. Current methods used to design the TPS decouple the flow phase from the material phase, hindering the capturing the physics at the interface and, therefore, cannot capture coupling effects between each phase.

The interactions between the aerothermal environment and the material response result in highly coupled, multi-physics problem and are key challenges in optimizing design margins and mission risk. The equations governing the Thermal Protection Material (TPM) phase are tightly coupled to the equations governing the flow field (the environment phase) at the interface of the two domains. Historically, three general strategies have addressed the flow/material coupling problem. In increasing order of fidelity, we can enumerate these strategies in terms of numerical solvers:

1) decoupled, standalone solvers for material and flow domains,

2) weak or strong coupling between standalone solvers, and

3) unified or one-domain solvers.

To consider both phases in the same computational domain, one must account for the multi-scale aspects of porous media structures. Since it is not feasible with current computational resources to resolve the macro and micro scale in the same domain, we must locally average the governing equations using Volume Average Navier-Stokes (VANS) equations [Wh199, QW1994]. The averaged equations are closed by employing effective transport properties. In this poster, we present the development of a one-domain VANS formulation for the conservation of mass and momentum for both fluid and porous phases, allowing intrinsic coupling between them. We have included the variable permeability across the interface of both phases derived in [Br2004], enabling the closure of the macroscale equations. Compared to a sharp permeability variation, the variable permeability closure significantly impacts the flow field macroscopic properties such as average velocity, pressure drop, and shear stress. For instance, we have predicted in-depth shear stress that the sharp permeability model cannot. This in-depth shear stress can induce mechanical removal inside the material, which is paramount to capture when designing TPS. Moreover, with this approach, one can estimate the jump coefficients between the pure fluid and a porous medium, enabling the closure of the boundary conditions derived by [OT1995] and [VP2013].

The finding of this poster shows the importance of modeling the flow and material in a unified manner and reveals essential aspects that previous coupling approaches cannot. The development of this one-domain model with a proper interface resolution allows for a higher fidelity assessment of TPS response, reducing design margins and mission risks. In the future, we intend to use the filtering approach from [Br2004] to derive effective properties for more complex microstructures relevant to aerospace applications.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS12 / 205

Simulation of the inelastic deformations of porous reservoirs under cyclic loading relevant for underground hydrogen storage

Authors: Kishan Ramesh Kumar[1]; Herminio Tasinafo Honorio[1]; Hadi Hajibeygi[1]

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Subsurface geological formations can be utilized to safely store large-scale (TWh) renewable energy in the form of green gases such as hydrogen. Successful implementation of this technology involves estimating feasible storage sites, including rigorous mechanical safety analyses. Geological formations are often highly heterogeneous and entail complex nonlinear inelastic rock deformation physics when utilized for cyclic energy storage. One of the major concerns of energy storage in the subsurface is the consequent ground surface subsidence or uplift. Several researchers in the past have reported subsidence in the carboniferous sandstone fields across the world which are used to produce hydrocarbons (Hettema et al., 2002; Teatini et al., 2011). When these reservoirs are used to store hydrogen, this results in seasonal cyclic loading on the reservoir that could cause permanent subsidence or uplift depending on the operating conditions and the rock characteristics. This calls for accurate modeling of subsidence for understanding the grain scale physics of the rocks in the subsurface. In this work, we present a novel scalable computational framework to analyze the impact of nonlinear deformation of porous reservoirs under cyclic loading. The proposed methodology includes three different time-dependent nonlinear constitutive models to appropriately describe the behavior of sandstone, shale rock and salt rock. Inelastic deformations such as plasticity observed in sandstone (Pijnenburg et al., 2019), viscoplasticity observed in shale (Haghighat et al., 2020) and creep in rock-salt (Spiers et al., 1990) are commonly observed in underground formations by these rocks.

To model creep, a power law formulation, where strain rate is a function of stress, was employed for brittle rocks (Bérest et al., 2019; Xu et al., 2012). To model plasticity of sandstone, cyclic modified cam clay model (MCC) (Carter et al., 1979) is further extended to account for viscoplasticity of shale rocks using a Perzyna based formulation (Haghighat et al., 2020). An implicit time-integration scheme is developed to preserve the stability of the simulation. Firstly, these models are implemented and compared with the existing literature. In order to ensure its scalability, the numerical strategy adopts a multiscale finite element (Ramesh Kumar & Hajibeygi, 2021) formulation, in which coarse scale systems with locally-computed basis functions are constructed and solved. Further, the effect of heterogeneity on the results and estimation of deformation is analyzed. Lastly, the Bergermeer test case –an active Dutch natural gas storage field comprising predominantly of sandstone– is studied to investigate the influence of inelastic deformation on the uplift caused by cyclic injection and production of gas. The constitutive laws are calibrated based on the uplift recorded by GPS stations for 1.75 years and then the uplift is compared with the GPS recorded stations for the remaining 2 years. The present study shows acceptable subsidence predictions in this field-scale test, once the properties of the finite element representative elementary volumes (REV) are tuned with the experimental data.

Participation:

In-Person

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207

Finite element simulation of four - dimensional geostress field under pressure flooding with different fracture network modes

Authors: Mingwei Jia[None]; Yongmao Hao[None]

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In the development process of low permeability reservoir, pressure flooding water will produce huge changes in pore pressure and stress conditions, thus leading to the opening of dynamic fractures. However, due to the difficulty of fracture microseismic monitoring and other factors, in order to clarify the morphology of fracture propagation after pressure flooding, the evolution law of in-situ

stress field and the formulation and optimization of reservoir reconstruction design will be provided with effective technical support. On the basis of one-dimensional geomechanics in a single well, the complex fracture network modeling method set up by rock mechanics and pumping program was used in this study to study the formation stress and pressure conduction law in high-pressure water injection process under different fracture network modes. Through complex fracture network modeling, the simulation method of geology, in-situ stress and fracturing coupling was adopted to propose the simulation method of pressure flooding "four-dimensional" in-situ stress field.The results show that with the pressure flooding and high pressure water injection, the three-way stress in the injection well increases and the three-way stress in the production well takes effect, but the horizontal two-phase principal stress in the plane shows obvious banded distribution along the respective stress directions. In the process of injection and production development, the horizontal principal stress difference is the largest in the horizontal well corresponding to the injection well, and the smallest in the unused area between the injection Wells.

Participation:

Online

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Energy Transition Focused Abstracts:

MS07 / 208

Upscaling and Automation: New Opportunities for Multiscale Systems Modeling

Authors: Ilenia Battiato[1]; Kyle Pietrzyk[1]

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Defense and energy applications ubiquitously involve multiscale and multiphysics systems. The accurate modeling of these systems, critical to achieve superior performances and optimized designs, has challenged generations of computational physicists due to the mathematical and numerical complexities involved in the development of their computable representations. One of the fundamental challenges associated with modeling multiscale processes is the development of rigorous models at the scale of interest (system-scale), which is typically much larger than the scale at which the physics is best understood (fine-scale). Coarse-graining techniques are a suite of mathematical strategies that allow one to perform rigorous scale translation, while bounding a priori upscaling errors. Yet, they require substantial time and mathematical expertise to use. This is due to the number analytical manipulations and rigorous approximations (e.g., series expansions) involved during model development that quickly become analytically intractable for systems of realistic complexities (e.g., systems with large numbers of interacting physics, nested scales, and chemical species). While computational physics has primarily focused on the aggressive advancement of numerical strategies for the solution of discretized PDEs of complex multiscale multiphysics systems, the applied mathematical techniques necessary for model formulation have continued to heavily rely on the speed and

mathematical skill of humans rather than machines. As a result, their application to systems of realistic complexities has been very limited. With this work, we suggest that combining upscaling and automation allows to go beyond human-centered limitations and to accelerate model development processes. In this talk we propose a method of automatic upscaling through symbolic computation. By streamlining the upscaling procedure and derivation of applicability conditions to just a few minutes, the potential for democratization and broad utilization of upscaling methods in real-world applications emerges. We demonstrate the ability of our software prototype, Symbolica, by applying it to thermal runaway in battery packs and reactive transport in large reactive systems.

Participation:

In-Person

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MS15 / 211

An Improved Pore-scale Rock-typing Method using Minkowski maps for the Sensitivity of Regional Support Size

Authors: Han Jiang[None]; Chaozhong Qin[1]; Christoph Arns[2]

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[2] *UNSW*

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The rapid advancement in digital core analysis has greatly promoted the research development of flow and transport in porous media. However, the field of interest revealing pore level information that can be processed through standard digital core analysis workflow is rather limited for practical purposes. The integration of pore-scale information into continuum scale is widely concerned as it associates deeply with the future development of digital core analysis. For hierarchical porous structure, pore-scale rock-typing and upscaling of petrophysical properties is a promising solution to bridge the gap between microscale and continuum scale. Morphological and topological parameters associating data clustering methods are popularly utilized for the pore-scale rock-typing on 3D digital samples. However, the size of regional support window through which the fields of the parameters are generated greatly affects the descriptive capacities of the parameters on the structural characteristics, thus the classification using traditional unsupervised clustering methods such as Gaussian Mixture Models (GMM) is hard to deliver optimal performance. Towards the issue, we propose in this work to apply a supervised method called Support Vector Machine (SVM) for rock type classification. Minkowski functionals are determined as robust descriptors for the morphological and topological characteristics of porous structures, and a fast computational method utilising Fast Fourier Transform (FFT) has been applied for the generation of the fields of the regional Minkowski measures. On the basis of the Minkowski fields generated through different regional support sizes from the target porous structures, comparative experiments between the two different classification

methods SVM and GMM have been conducted on two complex artificial porous systems and one digital image of a laminated sandstone. Throughout the tests, SVM has illustrated obvious advantage on overcoming regional support size effect even with limited labelling information. The combination of regional morphological and topological descriptors with SVM method could provide extraordinary convenience for the realization of pore-scale rock-typing on large 3D digital images with excellent computational efficiency.

Participation:

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MS08 / **212**

Cooling of CO2-rich geothermal fluids: A mechanism for cave systems formation

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Rock-groundwater interactions may substantially alter the shape and size of voids in the rocks comprising Earth's upper crust. In carbonate aquifers, these interactions often lead to intense dissolution and the formation of extensive karstic cave systems. Recent studies show that a large portion of the known karst systems was formed by groundwaters ascending from depth ("*hypogenic karst*") rather than by CO_2-loaded meteoric water that infiltrated from the surface ("*epigenic karst*"). The hypogenic karstic cave systems often make up giant and complex mazes of caves with passages reaching hundreds of kilometers and have significant hydrogeological implications. Despite the importance of the hypogene karstic cave systems, the mechanisms of their formation have remained elusive and ill-constrained [1-2]. To address this issue, we provide herein geological, geochemical, and theoretical evidence that many hypogene karst systems were most likely formed by the interaction of carbonate country rocks with CO_2-rich geothermal groundwater that rapidly ascended from depth. As the water cools, carbonate solubility increases (due to its retrograde solubility), inducing rock dissolution and cave formation on relatively short geological timescales. A numerical simulation based on this scenario produces maze-like hypogenic karst cave systems very similar to those observed in field studies and constrains the range of feasible hydrological, geological, and geochemical conditions. These conditions are very common in Earth's crust, suggesting that the scenario proposed herein for the formation of extensive hypogene karstic caves may be ubiquitous worldwide. Finally, we demonstrate the large and relatively rapid impact of these rock-groundwater interactions on the global CO_2 cycle.

Participation:

In-Person

References:

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MS06-A / 213

Simulation of CO2-Brine Primary Displacement in heterogeneous carbonate rocks

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Prediction of fluid flow in the subsurface is crucial for many applications, including environmental contaminant remediation and climate change mitigation. However, many challenges are involved, as seen in many carbon dioxide storage sites worldwide; the carbon dioxide has migrated away from the injection points much faster than predicted. This suggests that understanding the underlying mechanisms needs to be improved, especially for heterogeneous reservoirs. Rock heterogeneity at the submeter scale significantly impacts single and multiphase fluid flow properties and is an essential control of flow at larger scales. Incorporating real heterogeneous flow properties into reservoir characterization is crucial to modeling and predicting fluid flow in the subsurface successfully.

Digital rock techniques are disclosing new opportunities to improve fluid flow and transport predictions across scales. They aim to include laboratory-based characterization protocols to incorporate the effects of small-scale capillary heterogeneity into reservoir scale simulations. When coupled with a numerical simulator and an optimization routine, the upscaled relative permeability and capillary pressure curves, and the corresponding effective petrophysical parameters are estimated.

This paper discusses an upscaling workflow that combines special core analysis (SCAL) and pore network modeling (PNM) interpretations with long-core experimental and numerical methods to characterize heterogeneous carbonate rocks. In this study, the Estaillades carbonate is analyzed using a numerical history match of a long core flood experiment with the 3D saturation distribution as a matching target and the 3D capillary pressure characteristics as a fitting parameter. Throughout this workflow, the reservoir core-analysis practices are improved in such a way that could address rock heterogeneities. Furthermore, the relative permeability and capillary pressure uncertainty range quantified from the stochastic SCAL simulations are proven for an upscaling workflow from the SCAL samples to the long core samples.

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Poster / 214

Carbon sequestration in porous materials: Uniform CO2 flooding and reaction front

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Injection of a CO_2-rich phase into a porous material initially saturated with water solution (i.e., drainage) leads to CO_2 dissolution and mass-transfer into the resident water solution. As a result of the accompanying decrease in solution pH, the solid matrix can be in chemical disequilibrium and induce dissolution-precipitation reactions such as carbonation (i.e., carbonate mineral formation) on the wetted surfaces. In turn, the chemical disequilibrium leads to continued undersaturation and dissolution of CO_2 and a substantial net mass-flux from the CO_2-rich phase to the solution phase. Such immiscible drainage with mass-transfer is a scenario shared with major capture and/or sequestration systems, ranging from a carbonation in cement-based-materials [1] and in natural aquifers composed of ultramafic rocks (e.g., basalts) [2] to selective capture and separation in industrial porous materials [3] and to caprock integrity estimations in subsurface CO_2 storage [4].
Under certain conditions, viscous fingering instabilities can emerge from the initially planar front and develop to preferential flow pathways for the CO_2-rich phase. These flow pathways can then lead to a bypass of the bulk medium and eventually failure in substantial capture or sequestration of CO_2 methods [5]. In this study, using *in situ* CO_2 flooding experiments in a Portland cement-based mortar acquired using X-ray micro-computed tomography [6] and theoretical analysis of linear stability, we characterize the conditions for the emergence of viscous fingering. We find non-trivial effects of the mass-transfer term, which strongly depends on the degree of saturation. The results contribute to improving Carbon Capture and Storage (CCS) techniques in both natural and engineered porous materials and to the advancement of carbon-negative materials, which are crucial for mitigating climate change.

Participation:

In-Person

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Poster / 215

Microbially Induced Calcite Precipitation Treatment of Naturally Fractured Concrete: From Micro-Scale Characteristics to Macro-Scale Behaviour.

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Concrete is the most consumed artificial material universally, and its production is responsible for about 1.5% of the UK's greenhouse emissions (Hibbert et al., 2022). Concrete assets are often exposed to harsh environmental conditions, including exposure to seawater, freeze-thaw cycles and temperature cycles, leading to degradation of the matrix. Reducing the permeability of degraded concrete is key to minimising further deterioration in order to prevent the ingress of corrosive chemical compounds and limit carbonation. Calcite bio-mineralisation provides a novel alternative to established concrete repair techniques. Microbially Induced Calcite Precipitation MICP offers excellent penetrability (even into micro-fractures), excellent adhesion and the ability to improve mechanical properties as well as reduce permeability. Yet, previous studies for MICP applications have mainly focused on treatment methods which are impractical for in situ application. Furthermore, assessment of the extent of crack repair has typically been limited to visual assessment at the surface.
This study provides a comprehensive experimental and analytical investigation of MICP treatment of 3D fracture networks in degraded concrete with an emphasis on understanding the spatial distribution of calcium carbonate precipitated within the fracture networks. The experimental investigations were conducted on degraded concrete collected from the Ayrshire coast in Scotland. MICP treatment results showed successful repair of five fractured concrete cores, with two cores displaying 3 orders of magnitude reduction in permeability after only 3 treatment cycles. Additionally, Brazilian tests demonstrated recovery of up to 50% of the concrete's original tensile strength. Moreover, SEM-EDS analyses and X-CT imaging before and after MICP treatments provide insight into mineral localisation and the interactions between biologically induced precipitates and pre-existing salts within the concrete media. Finally, analytical studies based on an equivalent permeability model highlight the influence of fracture characteristics (i.e. fracture orientation, quantity, aperture, and morphology) on the efficiency of MICP treatments.

Participation:

In-Person

References:

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MS08 / 216

Modelling anomalous diffusion in semi-infinite disordered systems and porous media

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The spreading of Brownian particles in space, in a macroscopically one-dimensional domain, is described by a Gaussian law for the probability density function. But deviations from Brownian motion are widespread across disciplines, and diffusion frequently exhibits a power-law dependence $x^2(t)\ \ Kt$, in terms of the anomalous diffusion exponent and the generalized diffusion coefficient K (with physical dimension length^2/time). Examples of anomalous diffusion arise in charge carrier motion in amorphous semiconductors, passive tracer particle motion and molecular motor-driven motion in biological cells, motion of particles in crowded environments such as biological membranes or dense liquids, and transport in gels. And yet, in naturally occurring porous media such as soils and rocks, as well as in natural and engineered pore structures such as membranes and in catalytic systems, diffusion of chemical species is almost invariably modelled as a Brownian process in terms of Fick's law; these disciplines completely ignore the possible—or likely—occurrence of anomalous diffusion in such heterogeneous, disordered media. Here, we develop the continuous time random walk (CTRW) framework to anomalous diffusion (with no advective velocity component) in disordered and porous media. For an effectively one-dimensional, semi-infinite disordered system connected to a reservoir of tracer particles kept at constant concentration, we provide the dynamics of the concentration profile. We develop a formulation for the concentration profile $C(x,t)$ in a semi-infinite space for the boundary condition $C(0,t) = C_0$, using a subordination approach. From this, we deduce the tracer flux and breakthrough curve at a given distance from the tracer source. For the "residual" breakthrough curves, given by $1 - C(x,t)$, we demonstrate a long-time power-law behavior that can be compared conveniently to experimental measurements, which are currently in progress. For completeness, we also derive expressions for the moments in this constant-concentration boundary condition.

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Poster / 217

Modeling Solute Transport in Heterogeneous Media with Uncertain Architecture via Physics Informed Neural Networks

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Natural subsurface systems are often composed by multiple geomaterials, constituting the internal architecture of the system, characterized by uncertain spatial distribution. This leads to incomplete knowledge of the material properties. Here we address uncertainty arising from the lack of knowledge on location of boundary interfaces between geomaterials and their influence on physical processes, such as fluid flow and contaminant reactive transport. Investigating flow and transport features in porous media under such uncertainties have promoted the adoption of different PDE solvers. Machine Learning based PDE solvers are promising tools, due to the ability to acquire the solution over the whole spatial-temporal domain at once utilizing collocation points dispersed erratically over the domain, which gives such models a significant advantage over conventional time-stepping PDE solvers by eliminating the requirement for time-consuming processes such as space and time discretization. Here our focus will be utilizing Deep Learning based PDE solvers, where neural networks will establish the trial space for our state variable of interest, solute concentration, and being obtained via training on physics driven constraints.

To this end we leverage Physics Informed Neural Networks (PINNs) for the numerical solution of classical contaminant transport. These Machine Learning approaches are promising for using structured prior knowledge to build data-efficient and physics-informed learning machine. PINNs fall into the category of unsupervised or weakly supervised deep learning algorithms, and showed great performance for forward and especially inverse modeling purposes, where unknowns of a scientific problem such as full solutions of the corresponding PDEs, or parameters and boundary conditions respectively, can be inferenced using sparse measurements

In this contribution we will show the application of PINNs to the solution of contaminant transport problems in heterogeneous porous media, where results will be shown upon relying on some representative test cases, including transport in one- and two-dimensional media. We will start by addressing specific challenges that limit the application of standard PINN approaches in the presence of heterogeneous materials. Then we will show the performance of PINNs for the specific task, starting from algorithms recently developed in the scientific machine learning community. Notably, we employ domain decomposition methods for partitioning the PDE problem into several subdomains each modeled by a single sub-network. This strategy enables us to use PINNs for heterogeneous systems, while the solution continuity between the diverse sub-network models is maintained through imposing residual and flux continuity conditions via properly specified loss functions. Finally, we will discuss key pros and cons of PINNs approaches if contrasted with standard solvers.

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Energy Transition Focused Abstracts:

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Micro simulation of CO2 flow-induced fracture propagation in deep shale

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Deep shale gas (buried depth greater than 3500m) is a realistic field and an inevitable trend for shale gas exploration and development to achieve an important breakthrough, which is of great significance for creating a new field of shale gas exploration and development. Deep shale gas reservoirs are deeply buried and have high closing pressure. Water based fracturing fluid will bring problems such as water shortage, clay mineral expansion, and backflow water pollution. Therefore, it is urgent to develop more efficient and environment-friendly fracturing technology. Supercritical carbon dioxide (SC-CO2) can not only desorb methane from shale organic matter to improve oil recovery, but also be buried underground to mitigate the greenhouse effect. It is a promising substitute for water-based fracturing fluid. The deep shale gas reservoir is in the geological environment of high temperature, high pressure and high stress. The rock may change from elastic brittleness to ductile plasticity. During fracturing, the deep rock may have a large range of plastic deformation. The fracture propagation theory and method based on linear elastic fracture mechanics are no longer applicable. It is particularly important to study the fracture propagation process according to plastic fracture mechanics. The nano pores in shale are developed, the pore structure is complex, and the size of nano pores varies widely. The fracturing fluid flow process in the nano pores of shale will eventually affect the macro scale fracturing effect. Therefore, it is necessary to carry out research on SC-CO2 flow induced fracture propagation on the micro scale of deep shale based on hydro-mechanical coupling plastic fracture mechanics. The following defines a hydro-mechanical coupling model based on the Darcy-Brinkman-Biot method, which takes into account shale microscopic pore structure, different wettability of organic and inorganic pores, gas slip effect, confining pressure, plastic yield stress, anisotropic stress and other factors. We analyzed the potential advantages of using SC-CO2 as a fracturing fluid replacement, including enhanced fracturing and fracture propagation, increased methane desorption and carbon sequestration potential adsorbed in organic-rich parts of shale. It is found that with the increase of confining pressure, the cracking is faster and the fractal dimension of microcracks increases. The higher the plastic yield stress, the higher the SC-CO2 saturation adsorbed on the organic matter after methane desorption, and the greater the carbon fixation potential. In conclusion, deep shale reservoirs with higher formation pressure, the fracture shape is more complex and the fracturing effect is better. The shale reservoir with large plastic yield stress has high carbon sequestration potential, which is more suitable for using SC-CO2 as fracturing fluid substitute.

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MS04 / 221

Coupled numerical modeling of the China Mock-Up experiment for swelling clay barriers

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A notable part of active research on engineered barrier systems for the safe disposal of nuclear waste involves finding and understanding appropriate buffer materials. A buffer material which acts as a barrier between a nuclear waste canister and the surrounding host rock must possess certain properties, some as low-permeability, resistance to contaminant transport, ability to withstand high temperatures and pressures for extended periods of time etc. Bentonite is one such suitable candidate for a buffer material. Predicting the long-term behavior of bentonite under coupled THMC conditions remains a challenge. The behaviour of the Chinese GMZ-Na bentonite was investigated on a technical scale in the China Mock-Up experiment which yielded a significant amount of data on this material. The analysis of this experiment requires numerical models taking into account the coupled thermal, hydraulic and mechanical processes occuring in the bentonite.
We performed such numerical modeling of the China Mock-Up experiment using a monolithically coupled thermo-hydro-mechanical model for partially saturated swelling porous media with vapour diffusion and phase change phenomena implemented in the open-source numerical code OpenGeoSys-6 (OGS-6). The aim of this analysis is manifold. Firstly, to study thermal desaturation due to the waste-induced heating process as well as the subsequent resaturation by formation fluids. Secondly, to look at different representations of the boundary conditions for temperature, pore pressure as well as displacement and their impact on the results. To better represent the interaction of porous and non-porous materials, a recently implemented feature in OGS-6 allows for partial assembly of the matrices and thus, enables the user to deactivate a subset of the processes for some certain sub-domains. We tested the functionality of this feature and utilize it to represent the steel tank and insulation layer surrounding the bentonite blocks in the experimental setup which proved beneficial for the representation of the measurements.

Participation:

In-Person

References:

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MS12 / 222

A novel CPR/block preconditioning framework for two-phase flow simulations in porous media by mixed hybrid finite elements

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Efficiency and robustness of the linear solver is a fundamental need in multiphase flow models in porous media, as sequences of large ill-conditioned systems of linearized equations have to be repeatedly solved during fully implicit simulations. This is a computationally intensive task, whose performance is usually dominated by the boosting capabilities of the preconditioner accelerating a Krylov subspace solver. Although efficient physics-based preconditioning techniques exist, notably the multistage Constrained Pressure Residual (CPR) method and its variants, their robustness is often sensitive to the specific structure of the Jacobian matrix, which can be modified depending on the discretization scheme used for the set of governing PDEs. This is the case with the Mixed Hybrid Finite Element (MHFE) method, where element and interface pressure variables are introduced as main unknowns in addition to the cell-centered water saturation. The resulting Jacobian matrix is characterized by a 3×3 block structure that differs from the 2×2 structure of conventional TPFA-based discretizations, originally targeted by the CPR method. Applying this tool to the 3×3 block Jacobian is ineffective, as general-purpose AMG usually struggles with the 2×2 element-face pressure subproblem. In this work, we address this issue by introducing a block preconditioner at the local pressure stage to exploit its inner 2×2 block partition. The resulting technique, mixing block preconditioning with the CPR method, has been denoted as Block CPR (BCPR). An extensive testing phase, even on challenging realistic problems, shows the robustness, efficiency, and flexibility of the proposed framework.

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MS07 / 223

Coupled LBM-DEM model and its application to droplet impact on deformable porous media

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The dynamic behavior of multiphase flow in gas-solid-liquid mixture systems plays an important role in various applications of petroleum industry, biochemical processing, chemical and metallurgical industry, food technology, water treatment, and sub-seabed CO2 storage and its understanding can provide insights in various phenomena like rain deposition, landslides and degradation of heritage artefacts and buildings.

In this paper, we propose a numerical model to simulate such problems, coupling lattice Boltzmann and discrete element methods (LBM-DEM). A cascaded LBM is used to simulate the liquid-gas flow field using a pseudopotential interaction model for describing the liquid-gas multiphase behaviour. A classical DEM resorting to fictitious overlaps between the particles is used to simulate the multi-particle system. A multiphase fluid-solid two-way coupling algorithm between LBM and DEM is constructed. The model is validated by three benchmarks: (i) single cylinder particle sedimentation, (ii) single floating particle on a liquid-gas interface and (iii) self-assembly of three particles on a liquid-gas interface. Our simulations agree well with theoretical or numerical results reported in the literature.

Our proposed model is applied to simulate droplet impact on deformable granular porous media at pore scale. The dynamic droplet spreading process, the deformation of the porous media (composed of up to 1000 solid particles), as well as the invasion of the liquid into the pores within a wide range of impact Weber number are well captured. The droplet spreading dynamics on particles is compared to droplet impact on a flat solid surface. A scaling analysis is conducted to unify the two impact problems taking into account different fluid properties (viscosity), fluid-solid interaction (surface tension) and deformability of the substrate. An energy analysis allows determining the different mechanisms at play, showing the effects of kinetic and potential energy, surface energy and viscous dissipation.

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MS03 / **224**

A discontinuous approximation for modeling multiphase flow and transport in complex porous media structures

Authors: Jumanah Al Kubaisy[1]; Pablo Salinas[2]; Christopher C. Pain[1]; Matthew D. Jackson[1]

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The control volume finite element (CVFE) method is inherently flexible for modelling flow and transport in complex geological features such as faults and fractures. The finite element method that captures complex flow characteristics is combined with the control volume approach known for its stability and mass conservative properties. The classical CVFE approach exploits two meshes: the element mesh that represents the petrophysical properties element-wise and the control volume mesh, centered on the element vertices, representing the saturation solution in the medium. The discrepancy between those two meshes introduces inconsistency in the transport solution especially along material discontinuities or abrupt material interfaces.

In this work, we present an original discontinuous formulation based on the CVFE method for modeling multiphase flow and transport in porous media. We introduce the element pair $P_{1,DG} - P_{0,DG}$ denoting a linear discontinuous Lagrangian velocity approximation and an element-wise pressure approximation, respectively. The formulation enables the use of a single mesh that, in return, does not exhibit the inconsistency issues described earlier. We validate the method and demonstrate the effectiveness of the approach with numerical examples of complex fractures in highly heterogeneous domains.

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Experiment and simulation of quasistatic fluid invasion resulting in pressure-saturation (p-s) hysteresis

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During imbibition, fluid-fluid interface at the inlet of a constriction experiences an increase in capillary force that results in rapid fluid invasion known as Haines jump (Haines, 1930). During drainage, the interface gets pinned at the end of the constriction, which causes p-s trajectories to follow different paths during imbibition and drainage resulting in p-s hysteresis. In this work, we performed quasistatic two-phase flow experiments and simulations of cyclic imbibition and drainage to have a quantitative understanding of pore-scale processes resulting in pressure-saturation (p-s) hysteresis. We considered two different 2D Hele-Shaw cell setups: a capillary tube with a horizontal constriction (ink-bottle) and a heterogeneous porous media randomly populated by cylindrical obstacles. In both setups, drainage and imbibition are driven by quasitatically changing the pressure gradient between the inlet and the outlet of the domain. The experimental results were compared with the results from numerical model in OpenFOAM, which solves the Navier-Stokes equations employing volume of fluid (Hirt and Nichols, 1981) method to calculate the position of the interface and the continuum surface force (Brackbill et al., 1992) model to describe surface tension. For the ink-bottle setup, we observed that multiphase flow through a single constriction displayed the signature trait of p-s hysteresis, which depends innately on the cross-section gradient. The steeper the cross-section gradient, the more pronounced the p-s hysteresis, moreover, p-s hysteresis did not occur below a critical gradient. We derived an analytical solution to calculate the critical gradient and compared it with the critical gradient obtained from experiments and simulations. In heterogeneous porous media setup, we observed rapid fluid invasion and retention patterns in small pores during imbibition-drainage cycles, which give rise to hysteretic p-s trajectories. This comparative study will allow us to quantitatively link the pore-scale capillary physics to large-scale p-s hysteresis.

Participation:

In-Person

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Numerical Simulation of Fluid-structure Interaction Mechanism of Fractured Porous Media with Natural Fracture

Authors: Ying Shi[None]; Yuliang Su[None]

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Numerical Simulation of fluid-structure interaction mechanism of fractured porous media with natural fracture

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In tight oil reservoirs, complex rock mass consists of two different kinds of media porous media and fissured media. Natural fracture effect the seepage characteristics of rock mass. The interaction of the seepage field and the stress field forms the coupling of the stress field and the seepage field. During injection or production, the dynamic change of matrix and fracture will change the rock physical parameters. However, the experimental study cannot observe the rock deformation and fracture propagation.

In order to quantity characterize the distribution of natural fracture. This work used micro-CT to scan true core pore structure. The two-dimensional network model of porous media containing natural fracture models is extracted and reconstructed by analytical techniques. The fluid mechanics process in fractured media during fluid injection was simulated using COMSOL Multiphysics. The direct coupled method is employed in order to fully capture interactions between solid and fluid equations. Moreover, the indirect coupled method is employed to use the pressure function contacting material characteristics and constitutive equations of matrix and fracture. The natural fracture is traced by the level set of the joint element embedded in the adjacent finite element and the XFEM method. The ordinary finite element is used in the matrix, while the extended finite element is used in the fracture. The weak coupled separates the fluid from the solid, converts the load on the fluid domain into the deformation of the solid domain, and solves the fluid dynamic equation and the structural dynamic equation respectively. Fluid-structure interaction on the rock porosity and permeability are illustrated by a numerical experiment In addition, for testing the degrees of rock damage and fracture propagation during gas injection production. A sensitivity analysis of the Boit-Willis coefficient was performed to determine the degree of fluid-structure interaction. Two distinct Biot coefficients are designed for the matrix-matrix and the matrix-fracture system.

The result reveals the more inhomogeneous the stress field caused by fluid flow and the higher the damage degree of rock with the higher the Biot-Willis coefficient. This work reveals the fluid-structure interaction mechanism of natural fracture. The deformation of pore medium and fracture medium caused by different injection modes, the propagation of pressure in matrix-fracture and the change of reservoir rock physical properties are studied. This study reveals the mechanism of fluid-structure interaction effect on oil recovery during fluid flooding in tight sandstone reservoirs. Furthermore, the fluid-solid coupling mechanism of fractures is considered to gain a more realistic understand of the pore-scale phenomena and the fluid interaction between matrix-fractures and matrix-matrix.

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Adsorption behaviors of shale oil and water in mixed-wet pores

by molecular simulation

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Because shale matrix contains rich nanopore system and complex composition, it provides the necessary conditions for the existence of mixed-wet pores. Obtaining the adsorption behavior of shale oil in mixed-wet pores under water bearing conditions is of great significance for further understand the presence of shale oil in the reservoir from the mechanism. In this work, we constructed two types of kerogen-kaolinite nanopores (kerogen-gibbsite pore and kerogen-siloxane pore) using molecular dynamics simulations to study the adsorption behavior of shale fluids and the interactions between substances (fluid-wall and oil-water) in the system. The gibbsite and siloxane are two surfaces of kaolinite with opposite wettability.

In the kerogen-gibbsite pore, the presence of the water film not only compresses the effective space for shale oil to exist, but also aligns the polar part of the non-hydrocarbon components close to the water film by forming hydrogen bonds. This arrangement will make it easier for the non-polar part of the non-hydrocarbon component to capture the asphaltene in the shale oil, which will increase the chance of blocking the pores. In addition, by constructing kerogen-quartz pore to investigate the interaction energy and density distribution, we have confirmed that the existence of water film can almost completely shield the influence of hydrophilic inorganic wall on internal shale oil. With the strong hydrophilic properties of the gibbsite walls, water forms two types of hydrogen bonds with the hydroxyl groups on the walls. Therefore, the density distribution curve will form a small peak and an ultrahigh density peak region closest to the gibbsite wall. The calculated interaction energy shows that the H atoms divided in the small peak occupy 83.33% of the total water-wall interaction energy (Etotal), and all of it is the Coulomb interaction energy (Ecoul) under attraction. However, the O atoms in the water in the ultrahigh density peak are too close to the O in the wall due to the hydrogen bonding attraction and therefore the van der Waals force is repulsive.

In the kerogen-siloxane pore, the siloxane surface competes with kerogen for adsorption of internal shale oil. Although shale oil appears in regular multiple adsorption layers on the siloxane surface and the highest adsorption layer density is 2.12 times higher than the peak adsorption near kerogen, it is interesting to note that the amount and intensity of shale oil adsorption on kerogen remain higher than that on the siloxane surface. The effective oil-water contact surface area in both types of pores is an important factor affecting the interaction energy. When the water content is low, the oil-water contact surface area in the kerogen-gibbsite pore is larger than that in the kerogen-siloxane pore. On the contrary, when the water content is higher, the shale oil interacts with water more strongly in the kerogen-siloxane pore.

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Semi-analytical Solution of Multi-scale Transient Flow to a Horizontal Well Considering Micro-scale Lamellation in Shale Oil Reservoirs

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Microscale flow effect cannot be ignored in shale with a large number of organic/inorganic nanopores and microscale lamellar fractures. Due to multiscale flow characteristics, traditional Estimated Ultimate Recovery (EUR) evaluation methods are not accurate for assessing productivity in shale reservoirs. The flow model considering interaction among matrix with organic/inorganic nanopores, lamellar fractures and hydraulic fractures has not been established. This paper presents a semi-analytical model to characterize the multi-scale flow considering stress sensitivity in shale reservoirs.

Semi-analytical model of organic and inorganic nanopore, microscale lamellar fractures and complex fracture networks flow are established based on the linear flow. Diffusion, adsorption and slippage are considered in nanopores, as well as critical starting pressure gradients during flowing to inorganic nanopores. A fractal method is introduced to characterize hydraulic fracture spacing, porosity, and permeability. The multi-scale stress sensitivity is also considered based on the above characterization. Flow relationship among organic/inorganic nanopores, microscale lamellar fractures, and complex fracture network is described. The flow characteristics of shale oil are analyzed and accurately characterize the stress-dependent fracture properties (such as permeability and porosity).

We validate the semi-analytical model using production data from real shale oil wells and the predicted results agree well with the field data. The heterogeneity of induced fractures is considered in this model, and the sensitivity analysis shows that fractal distribution of fracture spacing has a larger impact on the interporosity-flow coefficient than that of the permeability and porosity. The stress sensitivity and compressibility of the three continuum are analyzed, the permeability loss of the matrix reach up to 15% and the permeability loss rate of the hydraulic fracture would be reduced by nearly 40% under the same compressibility and stress sensitivity, In terms of production, the contribution of the matrix in the later stage would be significantly reduced, but the overall production would be significantly increased.

Based on the model, dimensionless curves were constructed to analyze the productivity of horizontal wells in the field. It is also found that microscale effects such as diffusion, adsorption and slippage of nanopores and microscale lamellar fractures in the matrix has a great influence on production in the late time.

The novelty of this work is the introduction of a new mathematical model, which can comprehensively and efficiently characterize the multi-scale flow among matrix with organic/inorganic nanopores, microscale lamellar fractures, and complex fracture network in fractured shale oil reservoirs. It will be of great interest to operators seeking a quick method for production evaluation and prediction in shale with lamellar fractures.

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Saturated Mixing due to Reactive Viscous Fingering in Porous Medium

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The flows in porous media feature an interfacial instability, named viscous fingering (VF), that occurs when a fluid in a porous medium is displaced by a fluid with higher mobility. Various physical processes, such as petroleum Industry [1], carbon dioxide sequestration [2], and hydrology [3], to name a few, involve VF instability. A simple chemical reaction can modify the VF instability by modifying local viscosity distribution. To understand the chemo-hydrodynamic instability, we consider the radial displacement of two miscible and reactive fluids that undergo the reaction A+B⟶ C and generate a product with a different viscosity from the reactants. Convection and diffusion are two existing fundamental flow processes that compete with one another. By changing the viscosity profile, the product creation influences this competition and the VF instability [4,5]. By numerically integrating the convection-reaction-diffusion system of equations coupled with Darcy's law, we carry out non-linear simulations [4,6]. We demonstrate how the reaction amplifies instability while VF also enhances fluid mixing. We observe that if the reaction results in a product with a higher viscosity than the reactants, then the mixing in the system achieves saturation. Such finger patterns were referred to as frozen fingers [7].

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On the Influence of Permeability Variation and Viscous Fingering on Dispersion in Miscible Flow Displacements

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The interaction between viscous instability and the heterogeneity of the medium in a miscible displacements is interesting from many aspects. The problem is faced in various applications from contaminant transport to miscible oil displacement, carbon capture and storage, and polymer slug injection projects. Qualitative observations have shown that the length scale of heterogeneity has a prominent role in defining its contribution to hydrodynamic instability and thus mixing. The flow in a medium with a smaller length scale of heterogeneity behaves similar to the flow in a homogeneous porous medium. As the length scale of heterogeneity grows, its contribution to flow instability becomes more dominant. Many efforts have been made to analyze and quantify the observed effects in random heterogeneity models, however such analyses are case dependent and hard to generalize. Thus simpler models of heterogeneity have been adopted for understanding the fundamental mechanisms of spreading and mixing in unstable miscible displacements. In numerical investigations of miscible displacements through evenly distributed layers, with the width of the layers w defining the length scale of heterogeneity, the dominance of each of the instability mechanisms have been found to be a time dependent concept. Mixing in such media, represented by mixing zone length, MZL, follows four flow regimes: an initial diffusive flow regime, channeling regime (heterogeneity dominated instability), lateral diffusion (a second diffusive flow regime), and viscous-fingering-dominated regime. The mixing during the second diffusive flow regime, driven by diffusion of the grown fingers across the high permeability layers, shows a dispersive behavior, growing linearly with the square root of time but at a higher rate than the first diffusive flow regime. In the current work the effect of heterogeneity and viscous fingering parameters on the effective dispersion rate during this regime has been investigated.
A miscible displacement in a Hele-Shaw cell with harmonic permeability variation across the flow channel has been modelled using a fully implicit spectral method. According to the numerical simulations, for given pair of fluids the effective dispersion coefficient is proportional to the square of the heterogeneity length scale. The effects of different values of viscosity ratio, M, and strength of heterogeneity, s, on dispersion rate are more complex to quantify. It has been observed that while the rate of dispersion is affected by the mobility ratio or the heterogeneity variance, the time of transition between the channeling and the lateral diffusion regimes is independent of these mechanisms. It is concluded that the diffusive time scale $\tau_D=w^2/D$, defines how long the channeling regime lasts, and the flow convection, the permeability variation, and the unfavorable viscosity ratio, collaborate to form and grow instabilities during this enforced time period. Larger values of Pe, M, and s, result in enhanced instabilities formed at the start of the dispersion dominated regime and a higher effective dispersion due to the larger contact surface between the solute and the inhabitant fluid.

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A molecular dynamics study on dissolution and adsorption dynamics of CO2 with H2 impurity in oil reservoir

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CO2 capture and storage (CCS) is one of the indispensable decarbonization technologies to achieve green industrial growth and address the challenge of global climate change. CO2 captured using the Sorption Enhance Water Gas Shift process at steel mills contains H2, with its molar ratio reaching 10% or higher. Since the thermophysical properties of CO2 and H2 are distinctly different, the effects of H2 impurity on CO2 transportation and geostorage in oil reservoir should not be overlooked. Moreover, according to our previous modelling study, the solidification of oil on caprock surface can generate a preferentially orientated molecule structure because of the interfacial crystallization. The solidified oil film can alter the minimum miscible pressure of the gas mixtures, thereby changing the adsorption and dissolution process of CO2 in oil reservoir.
In this study, molecular dynamics simulation will be performed to investigate the effect of injection temperature and pressure on the dissolution behaviour of CO2/H2 mixtures in solidified oil film. The crystalline alkane structure on silica subtract will be constructed, featuring the surface freezing monolayer and the crystalline parallel middle layers. The atomic interaction energy between the gases, function groups of alkane and silica subtract will be quantified to elucidate the mechanism behind the miscibility and surface adsorption. The conclusion of this study will shed guiding light on optimising the operating conditions of injecting CO2 containing H2 as the major impurity species and facilitating the deployment of CCS infrastructures.

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A sensitivity analysis on the performance of geothermal heat exchangers implemented in abandoned oil and gas wells

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With the growth of population and various industries around the world the demand for energy has increased rapidly. The use of fossil fuels as the main source of energy is considered a threat to the

environment due to the release of large amounts of carbon dioxide in the atmosphere resulting in global warming and climate change. Geothermal energy is one of the potential energy sources with low-carbon footprint that has been used to generate electricity since the 20th century. Geothermal energy extraction systems involve water as the energy carrier and the subsurface layers' higher temperature as the main source of energy. The costs of drilling to reach the depths with economically viable temperature are considerable and one of the obstacles against extensive use of this source of energy. Therefore reuse of abandoned oil and gas wells has been considered lately as a more economic option. Unlike the open loop circulation systems encountered in conventional geothermal reservoirs and enhanced geothermal systems, the double pipe heat exchanger set-up in and abandoned cased well, forms a closed loop heat exchanger with a more environmental friendly arrangement. For these systems an inner pipe with a smaller diameter than the casing is placed in the well coaxial with the casing. The water is injected into the annulus and its temperature increases as it moves towards the bottom of the well. Next, the hot fluid enters the inner pipe and moves upwards to reach the well head. The efficiency of the energy harvesting process, and thus a potential well's appraisal, highly depends on the outlet water temperature. In turn the outlet temperature depends on the well and the formation's thermal properties along the well which is hardly available and adds to the uncertainty of the assessments.
In this study, a comprehensive sensitivity analysis has been conducted on coaxial heat exchangers and the role of the well and formation's thermal characteristics, fluid's thermal and hydraulic properties, and the operational parameters such as the inlet fluid temperature and its injection rate, on the output well temperature has been investigated. For this purpose, a dataset based on the Latin hypercube method has been created using a three dimensional proxy model built in Opengeosys software. The correlation between the output temperature and the 16 involved parameters has been investigated through six statistical analysis methods including Pearson correlation coefficient, maximal information coefficient, linear regression, decision tree regression, random forest regression and xg-boost regression. A comparison between the linear and nonlinear regression methods has shown that the nonlinear methods do not necessarily add to the accuracy of the regression. The final ranking of the parameters has been performed based on the overall result of these analysis methods. The 8 more important parameters (ordered with respect to their importance) have been found to be the well depth, the inlet fluid temperature, the geothermal gradient, the fluid flow rate, the fluid's specific heat capacity, the formation thermal conductivity, the inner pipe thickness, and the outer pipe thickness.

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Poster / 245

Permeability Contribution Estimation of Different Pore Structures in the Heterogeneous Porous Media Using Image-Based Rock Typing

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Quantitatively estimating the permeability contribution of different pore structures in a heterogeneous porous medium plays a crucial role in assessing the influence of some diagenesis such as intragranular erosion and clay cement on the reservoir permeability. This study proposes an effective method to estimate the permeability contribution of a specific pore structure in a heterogeneous rock sample via six steps. First, the image-based rock typing is implemented to classify a multiscale pore structure into different rock types where each rock type presents a homogeneous pore structure, using the random forest algorithm. Second, the 3D model of the macropore structure and every micropore structure is reconstructed applying the MPS method. Third, the permeability of each reconstructed 3D micropore structure is calculated using LBM, and the corresponding permeability REV of this structure is estimated. Four, an upscaling process is carried out to divide the reconstructed 3D macropore structure into many cells whose length is determined by the maximum permeability REV of the micropore structures. Five, the permeability of every cell of the coarse grid is calculated by LBM except some cells that are randomly selected as micropore structures whose permeability is assigned directly according to their rock types. Finally, the permeability contribution of each micropore structure is evaluated by comparing the permeability calculated before and after assuming the target micropore structure is impermeable. The result shows that the permeability contribution of a micropore structure varies significantly according to its permeability, content, spatial distribution, and the permeability of the macropore structure.

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In-Silico Screening of CO2 Diffusion and Ions Distribution in Porous Media

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The ubiquitous behavior of thin film brine residing in mineral pores confined by mineral and oleic phases fascinates many porous media researchers [1–4]. The unusual behavior of an aqueous phase

in confining systems is dominated by a broad range of sciences, from drug delivery and catalytic reactions to enhanced oil recovery. So far, extensive efforts have been pursued to unveil the underlying mechanisms behind the stability of thin film brine covering the surface of porous media, mainly by tuning the salinity, which changes the wettability of the porous media surface. In addition, finding an efficient way to eliminate carbon dioxide in the environment has gained attention [5, 6]. Carbonated Low Salinity Water (CLSW) has been introduced to achieve these common purposes. In this study, molecular dynamics simulations have been performed to unravel the influence of CO2, salinity, and the polar component of the hydrophobic phase confined in an identical porous medium. The confined CLSW thin film (40000 and 8000 ppm of NaCl) between a calcite substrate and a hydrophobic fluid, consisting of decane, and acid molecules, benzoic acid (BA) or decanoic acid (DA) at high pressure and high temperature (HPHT) conditions (323 K and 10 MPa) has been investigated. Atomistic simulations reveal that the compacted, well-ordered layers of water in the proximity of the calcite substrate are formed regarding the salinity and the component of the oleic phase. The diffusivity of CO2, acidic molecules, and ions have been changed upon changing the salinity and oil model. The polarity of the BA and DA functional groups, and water ions, makes the interactions more complicated. The higher acidity of DA compared to the BA makes it a better case to move toward the brine phase. At the same time, a higher interaction of carbon dioxide with BA than DA was seen. The higher interaction of BA by CO2 impedes the higher diffusivity of CO2 into the oleic phase compared to the DA. However, the chain structure of DA makes the space accessible for the diffusion of CO2 into the oleic phase and distribution into the bulk oleic phase, which results in higher interaction of decane and lower viscosity for this model oil. Also, the higher diffusion of DA compared to the BA proves the idea of a higher attraction of Na+ ions toward the DA than BA, which would end up with a thicker electrical double layer over the calcite surface. Overall, the attraction of Na+ ions toward the calcite substrate will decrease by introducing DA instead of BA in the system, and it prefers to move toward the oleic interface. In lower salinity, the higher interaction of CO2 with acid molecules has been seen, particularly in the BA case, which indicates that the ions are not enough to move to the interface and trigger the interaction with acidic molecules. Therefore, the accurate oil composition, along with the brine salinity, should be considered in the screening procedure of the carbonated water implementation.

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3D modeling of macro-segregation and formation of freckles in solidification based on the fully decoupled enthalpy-porosity method

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The problem of solidification with macro-segregation and the formation of freckles is usually a complicated one that involves mass, momentum, heat, and species transfers between the solid, mushy, and liquid phase regions [1]. In several natural and industrial applications, the quantitative description of phase change, chemical heterogeneities, and multi-phase and multi-component flows serve an essential role in this process. In the aerospace industries and civil engineering, where materials with high strength, heat-treatable capacity, and fatigue resistance are in high demand, this naturally sets very strict requirements for internal compositions and their distribution in parts and workpieces [2]. For the petroleum industry, the efficient and economical recovery of natural gas hydrate from the subsurface and the safe operation of natural gas pipelines to prevent hydrate or wax blockage are also based on a deeper understanding of solidification and phase change [3,4]. Even on an interstellar scale, the deposition of planetary components during cooling constitutes a kind of separation [5]. Nonlinearities and interactive multi-physical fields are the major challenges in modeling this topic, and they raise the high computational costs associated with its 3D simulations. Our work proposes an operator-splitting and matrix-oriented method based on the enthalpy-porosity model to avoid non-linear systems. Also, the combination of vectorization and forward techniques to assemble the matrix of the linear system enhances the implementability of extensions to 3D applications. Finally, a number of 2D and 3D benchmark cases are presented to validate the accuracy and effectiveness of this scheme [6-8]. This numerical method also shows its ability to capture physical processes, such as channel segregation and freckle formation, caused by solutely and thermally driven flow.

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Propagation law of high pressure water injection in low permeability reservoir

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The phenomenon of “no injection or production” is common in water injection development of low permeability reservoir, which is one of the difficult problems restricting the efficient development of low permeability reservoir. It is urgent to explore effective injection and production mode to greatly improve injection capacity and development effect. After pressure flooding, the energy recovery of the well is good, but there are problems such as short effective time and difficult to balance the effect, so it is necessary to carry out regulation strategies for typical well groups. This paper intends to establish a fracture-propagation and seepage numerical simulation method for pressure flooding development based on fluid-structure coupling, clarify the morphology of water injection fracture network in pressure flooding, clarify the propagation and distribution law of pressure and media front during pressure flooding production, and put forward a long-term balanced and effective control strategy for pressure flooding, providing technical support for improving the pressure flooding development effect in mines.

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Energy Transition Focused Abstracts:

MS23 / 251

Comparison of two optimization approaches in an electrochemical reaction-diffusion system from an entropy generation perspective

Authors: Mehrzad Alizadeh[1]; Patcharawat Charoen-amornkitt[2]; Takahiro Suzuki[1]; Shohji Tsushima[1]

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As the use of electrochemical energy devices, such as rechargeable batteries and fuel cells increases in many fields, from stationary power generation to transportation and heavy-duty applications, it is imperative to further improve them to make them cost-effective compared to conventional systems [1]. The search for the best composition for porous electrodes of these technologies has been the interest of many researchers over the past decades. Recently, some studies, such as [2, 3], have focused on the use of topology optimization techniques in designing the electrode structure. While such studies provide beneficial techniques for innovative electrode design at the application level, fundamental understandings of the physicochemical mechanisms that improve system performance are strongly needed. This study fills this research gap by linking an optimization problem to the concept of entropy generation.

This study aims to investigate the optimal structure of an electrochemical reaction-diffusion (ERD) system. It is assumed that the proposed porous reactor consists of three material constituents, including a solid phase, a proton-conducting polymer (ionomer), and voids. Such a system is analogous to the catalyst layer of a polymer electrolyte membrane fuel cell. However, the method used in this study can be employed for any other type of electrochemical device with some slight modifications. A reactant species diffuses into this ERD system through the pores as it oxidizes in the presence of the solid phase. The solid phase and ionomer phase are responsible for discharging the generated electrons and positive ions, respectively. Two topology optimization strategies are used to find the optimal spatial distribution of constituent materials. In the first approach, the goal is to maximize the overall reaction rate in the system. In the second strategy, an attempt is made to minimize the losses of the system while keeping the overall reaction rate constant. An entropy generation model is developed based on the concept of non-equilibrium thermodynamics. The change in entropy production rate during the two optimization processes is evaluated and compared. The results show that both optimization approaches lead to a complex tree-root-like structure. Such a structure facilitates the delivery of reactant species to entire parts of the ERD system, thus reducing mass transport limitations. In addition, the findings of this study indicate that the entropy production rate increases with the increment of the total electrochemical reaction rate. This is associated with the increase of inevitable entropy production in a maximization approach. On the other hand, the minimization approach leads to lower entropy production, which is consistent with the minimization of entropy generation [4].

Acknowledgments
This work was supported by Grant-in-Aid for JSPS Fellows number 22J20603, JSPS KAKENHI Grant number 21H04540 and Office of the Permanent Secretary, Ministry of Higher Education, Science, Research and Innovation (OPS MHESI) (Grant No. RGNS 65-084), Thailand Science Research and Innovation (TSRI) and King Mongkut's University of Technology Thonburi.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 252

Entropy generation analysis in a quasi-3D PEM fuel cell model with architectured electrocatalyst layer

Authors: Mehrzad Alizadeh[1]; Patcharawat Charoen-amornkitt[2]; Takahiro Suzuki[1]; Shohji Tsushima[1]

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As the world grapples with global warming and other environmental problems caused by the extensive use of fossil fuels, a rapid shift to renewable resources is essential. The intermittent nature of solar and wind energies, the two main renewable energy sources, is a bottleneck to the widespread use of these sustainable energies. Deployment of electrochemical energy devices might be a remedy for this issue. The polymer electrolyte membrane fuel cell (PEMFC) is an efficient technology that converts the chemical energy of hydrogen into electricity through an electrochemical reaction. PEMFCs application includes but not limited to power generation systems, transportation, and heavy-duty applications [1]. Topology optimization (TO) has attracted much attention to improve the performance of various electrochemical systems [2, 3]. Compared to other mathematical optimization techniques, such as size and shape methods, TO is a more robust and stronger algorithm. The superiority of TO stems from the fact that it provides more freedom in achieving innovative design solutions. Recently, some researchers have focused on utilization of TO to improve the performance of electrochemical devices by controlling the microstructure of their porous electrodes [4]. However, far too little attention has been paid to the fundamental explanations of how improved performance is achieved through engineered electrode structure. This study attempts to provide a fundamental explanation by examining the changes in entropy production during the optimization process.

To accomplish the aims of this study, the performance of a PEMFC is first simulated based on a quasi-3D mathematical model. Next, a TO algorithm is recruited to find the optimal structure of the electrocatalyst layer with the purpose of increasing the output power density. An entropy generation model is developed to quantify the entropy generation rate during the optimization process. The entropy generation rate of the initial uniform design and the final architectured structure are compared to elucidate the fundamental mechanisms that lead to a better design.

Acknowledgments
This work was supported by Grant-in-Aid for JSPS Fellows number 22J20603, JSPS KAKENHI Grant

number 21H04540, and Research Strengthening Project of the Faculty of Engineering, King Mongkut's University of Technology Thonburi.

Participation:

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Poster / 254

An Upscaled Modeling Framework for Reactive Transport: A Case Study - Dry Creek, Idaho

Authors: Zachary Sherman[1]; Kevin Roche[2]; Thomas Sherman[3]; Diogo Bolster[4]

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Rivers and streams are important for transporting minerals, nutrients, and other chemicals throughout the natural environment. Introducing potentially toxic species into local water systems, e.g. agricultural-based pesticides, may have negative ecological consequences. Hence, understanding how materials are transported in hydrologic systems is important for developing more sustainable water management practices. The goal of this research is to validate a mathematical model that faithfully captures the transport of a reactive solute plume in a turbulent open channel with hyporheic exchange. To this end, field scale conservative (NaBr) and reactive tracer (NaNO3) experiments were conducted in Dry Creek, a small tributary in the Boise River watershed located in Idaho, USA. Reactive and conservative tracers were (pulse) injected into Dry Creek, and breakthrough curves were measured at 5.27m and 70.64m from the injection site. Here, we present analysis and results of the field study, linking creek characteristics to transport behavior. Then we develop a upscaled linear-reactive transport model using a CTRW framework to validate field study results. We compare the upscaled mathematical modeled breakthrough curves with observational measurements and use model insights to characterize the underlying governing process of reactive transport at the reach-scale. Specifically we explore the impact of the underlying sediment bed on channel transport in both the reactive and conservative cases.

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256

A comprehensive evaluating of acid-rock interaction induced shale pore structure change by fractal parameters

Author: Sai Xu[1]

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Adding acid to fracturing fluids is a promising method to for enhanced stimulated shale reservoir volume. The mechanical and petrophysical properties of reservoir are modified due to acid-rock interaction. It is of great significance to comprehensively understand the pore structure change behind the macro-performance alteration, for the purpose of maximizing the effect of acid-rock interaction in long-term productivity and ultimate recovery enhancement. In this work, low-pressure N2 adsorption and X-ray micro-computed tomography (micro-CT) scanning experiments are used to detect the shale pore structure change after acid-rock interaction. Base on the N2 adsorption isotherms, fractal dimensions are determined to quantify the effect of acid-rock interaction on nano-pores in shale, in terms of pore size distribution and pore surface roughness. Fractal dimensions are also calculated from CT images to estimate the change of micro-pore distribution. Moreover, the change of heterogeneity, anisotropy, and connectivity of micro-pores in shale are discussed in depth. The results show that acid-rock interaction reduces the surface roughness of nano-pores in shales. Shales with different mineral composition presents distinct change of nano-pore distribution. The dissolution of reactive minerals creates many micro-pores and fractures with different sizes, which leads to the increase in micro-pore distribution fractal dimension. Meanwhile, the increase in normalized lacunarity and succolarity demonstrates that shale pore structures become more heterogeneous and have better connectivity after acid-rock interaction. Porosity, fractal dimension, lacunarity, and succolarity are complementary parameters, and help to understand the pore structure change of porous media more comprehensively.

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Energy Transition Focused Abstracts:

MS03 / **257**

Numerical simulation of hydroshearing in fractured crystalline rock at the Bedretto Underground Laboratory (Switzerland)

Authors: Iman Vaezi[1]; Andrés Alcolea[2]; Peter Meier[2]; Francesco Parisio[1]; Jesus Carrera[1]; Victor Vilarrasa[3]

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Hydroshearing, or shear stimulation, is recognized as the main method to exploit geothermal energy in hot low-permeability crystalline rocks at depth. It consists of enhancing permeability via injection-induced shear slip and dilation of preexisting fractures. Hydroshearing usually causes some induced microseismicity, sometimes of sufficient magnitude to be felt on the surface. Thus, high-pressure fluid injection to enhance fracture permeability should be made carefully to avoid inducing earthquakes above the acceptable magnitude.

The process of hydroshearing is theoretically well understood and numerical models are capable of simulating it. However, fundamental investigations at the field scale are limited. This study focuses on the modeling of a hydraulic stimulation carried out at the Bedretto Underground Laboratory for Geosciences and Geoenergies (BULGG), in Switzerland, to investigate hydro-mechanical coupled processes due to fluid injection into fractured granite. We examine three numerical models with increasing complexity (a model with calibrated time-variable permeability, a model with strain-dependent permeability, and a model incorporating viscoplasticity with strain weakening and dilatancy) to improve the simulation and capture the hydro-mechanical response of the fractured rock mass.

The first model yields a reasonable fitting to measured overpressures at the injection borehole. Yet, the pore pressure distribution and the corresponding poromechanical response of the rock are not well captured. Employing an embedded model to calculate permeability changes as a function of volumetric strain improves the temporal evolution of overpressure at the injection borehole at the early stages of stimulation, but overestimates it once the fracture undergoes shear slip. Using a viscoplastic constitutive law with strain softening and dilatancy results in an additional enhancement of fracture permeability and thus a better reproduction of the monitored overpressures. The results show that the timestamps of monitored microseismic events correlate well with the times when permeability enhancement surpasses the previously maximum amount in each injection cycle.

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MS04 / **258**

Pattern Formation in Crumpled Hydrogel upon Rapid Dehydration with Acetone

Author: George Fortune[1]

Co-authors: Merlin Etzold [2]; Stuart Dalziel [1]; Julien Landel [3]

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It has been previously observed that when polymer gels (e.g. hydrogels) undergo rapid extensive swelling, a transient crumpling instability can form on the surface of the gel. This instability consists of many line segments of cusps patterning the gel's surface into an array of bumps that arise from shear bending of a homogeneously swollen gel surface

Here, we present experiments showing that when a hydrogel sheet whose upper surface exhibits such an instability is rapidly dehydrated (e.g. through rapid immersion in acetone), the instability is locked in place, becoming much visible as the bumps undergo a phase transition and change colour from transparent to white (see the attached figure showing this pattern for a range of initial water drop volumes). We explore the different facets of this rich behaviour, comparing the acetone induced pattern with the initial crumpling instability. In particular, we demonstrate that the pattern that emerges is independent of the total size of the blister, rather it is just a function of the time before immersion in acetone. Furthermore, by controlling the time before immersion we can control reliably the wavelength of the instability. We close by discussing potential next steps to be taken in investigating this fascinating phenomena.

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Energy Transition Focused Abstracts:

MS06-B / 259

Pore-scale mass transfer model of capillary trapping dissolution based on Sherwood, Reynolds, and Schmidt number

Authors: Anindityo Patmonoaji[1]; Yingxue Hu[2]; Tetsuya Suekane[3]

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Dissolution mass transfer of trapped phases in porous media is an important phenomenon in various fields, such as groundwater contamination [1–3], groundwater remediation [4], geological carbon sequestration [5], and energy storage in geological formation [6]. In the process of dissolution mass transfer, a fluid, which could be a liquid, gas, or supercritical fluid, is trapped in porous media by a capillary force. In the presence of another flowing fluid the trapped phase then gradually dissolves with solubility as the driving force.

The difficulties in investigating this phenomenon is the method to observe the dissolution process inside the porous medium. Earlier studies were mainly conducted using upscaled mass transfer approaches [1–4], which was modeled as a single grid block of mass transfer without knowing the pore scale processes in the porous media. As a result, the interfacial area, which the place for the mass transfer to occur, was unknown. For that reason, the developed mass transfer models [1–4] were phenomenological to the porous media.

In this work, we used X-ray CT microtomography (micro-CT) to observe the pore-scale process of dissolution mass transfer inside a porous medium. The main goal of using the micro-CT is to measure the capillary trapping interfacial area during the dissolution process, and thus, mass transfer model that is non-phenomenological to the porous media characteristics can be developed. To generate the mass transfer model, we performed comprehensive experimental investigations [7–12] by using various porous media characteristics (unconsolidated porous media particle size and wettability), various trapped phase types (non-aqueous phase liquids (NAPLs) and gases), and various water velocity.

Along with the development of this models, additional phenomena that affect the mass transfer rate were elucidated. The first phenomenon is the dissolution fingering [9], which occur due to slight differences in local permeability caused by the spatial distribution of the trapped phase in the porous media. Dissolution fingering was found to reduce the mass transfer coefficient to a third. Another phenomenon is the two-stage dissolution process [7,8] that occurs due to the rapid dissolution rate of the capillary trapping represented by the dissolution ratio (ratio between solubility and density). As a result, dissolution occurs much faster than the solute advection, resulting in the accumulation of high local solute concentrations that hinder the mass transfer process.

Eventually, a non-phenomenological mass transfer model based on Sherwood, Reynolds, and Schmidt numbers was developed. To the best of our knowledge, this is the first non-phenomenological model of capillary trapping dissolution mass transfer based on Sherwood, Reynolds, and Schmidt numbers. We believe that this work could provide valuable insights for the porous media community, especially interfacial phenomena across scales.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS20 / **260**

Anomalous transport in brain microvascular networks

Authors: Florian Goirand[None]; Tanguy Le Borgne[1]; Sylvie Lorthois[2]

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Blood microcirculation supplies neurons with oxygen and nutrients, and contributes to clearing their neurotoxic waste, through a dense capillary network connected to larger tree-like vessels. This complex microvascular architecture results in highly heterogeneous blood flow and travel time distributions, whose origin and consequences on brain pathophysiology are poorly understood. Here, we analyze highly-resolved intracortical blood flow and transport simulations to establish the physical laws governing the macroscopic transport properties in the brain micro-circulation (Goirand et al. Nature Communications 2021). We show that network-driven anomalous transport leads to the emergence of critical regions, whether hypoxic or with high concentrations of amyloid-β, a waste product centrally involved in Alzheimer's Disease. We develop a Continuous-Time Random Walk theory capturing these dynamics and predicting that such critical regions appear much earlier than anticipated by current empirical models under mild hypoperfusion. These findings provide a framework for understanding and modelling the impact of microvascular dysfunction in brain diseases, including Alzheimer's Disease.

Participation:

In-Person

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Goirand, F., Le Borgne, T., & Lorthois, S. (2021). Network-driven anomalous transport is a fundamental component of brain microvascular dysfunction. Nature communications, 12(1), 1-11.

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Energy Transition Focused Abstracts:

MS01 / **261**

Impact of capillary pressure hysteresis on Underground Hydrogen Storage

Authors: Farzaneh Nazari[1]; Shokoufeh Aghabozorgi Nafchi[2]; Rouhi Farajzadeh[3]; Vahid Niasar[4]

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The decarbonization of energy mainly requires the substitution of fossil fuels with low-carbon alternatives. Heavy industries require high-temperature heat that cannot be supplied through electricity. Moreover, the production of renewable electricity requires a storage medium to compensate for their intermittent behaviour. Hydrogen is a favorable medium for storing the excess low-carbon electricity and can accommodate the high temperature requirements. Subsurface hydrogen storage provides the mean to safely store and re-use the hydrogen gas. A successful storage project requires accurate modeling of the hydrogen movement and the extent of its loss.

Flow of hydrogen in porous media containing water is affected by hysteresis in flow properties, mainly relative permeability and capillary pressure. This hysteretic behaviour is a consequence of changes in contact angle and capillary trapping of non-wetting phase in porous media. As a result, the amount of hydrogen trapped in underground increases overtime, causing significant hydrogen loss. Most of the available literature have only considered the hysteresis in relative permeability and have not studied the path dependency of capillary pressure. Moreover, studies focused on the impact of hysteresis on hydrogen storage and hydrogen loss due to trapping is still scarce.

The overall aim of this study is to model the hysteresis effect during the two-phase flow of hydrogen-brine. The outstanding contribution of this work would be considering the capillary pressure hysteric behaviour through generating the full scanning curves during the injection/production cycles for each grid cell. At the next stage, we will look into the relative permeability hysteresis to investigate their individual and mixed influence on the hydrogen trapping in subsurface. Finally, we aim to perform a sensitivity analysis on the controlling parameters (rates, shut-ins and so on) to derive the most optimized scenarios for a successful storage operation. Due to the cyclic nature of the system, we speculate hydrogen loss because of increased trapped hydrogen during the consecutive cycles. We also expect the capillary pressure to be a less contributing parameter compared to relative permeability as the field-scale nature of the system is less affected by capillarity [1].

Participation:

In-Person

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MS06-A / 262

Derivation of 2-Phase Darcy Equations from Pore Scale Energy Dynamics using Non-Equilibrium Thermodynamics

Authors: James McClure[1]; Ming Fan[2]; Steffen Berg[3]; Ryan Armstrong[None]; Carl Fredrik Berg[4]; Zhe Li[5]; Thomas Ramstad[6]

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The upscaling of 2-phase flow in porous media from pore to Darcy scale is a long-standing problem. While several approaches have been published in the literature, there remains no consensus on what the right approach is and what the correct Darcy scale transport equations are. Many approaches assume explicitly or implicitly that a length scale exists where pore scale dynamics average out such that equipartitioning of energy in the different degrees of freedom holds, which is sometimes referred to as the multi-phase representative elementary volume (REV). The implicit assumption is ergodicity where spatial, temporal, and ensemble averages are equivalent.
Many theoretical approaches explicitly require ergodicity, and few general strategies have been advanced to treat non-equilibrium thermodynamic behavior associated with non-ergodic systems. We develop a non-equilibrium theory using time-and-space averaging; assuming that ergodic conditions hold only at very small length scales. For instance, at late times Haines jumps travel beyond the range of diffusive mixing (which would be required for equipartitioning). Since the timescale for mixing is fast at small length scales, many non-ergodic systems can be described based on this approach. We show that fluctuations are constrained by the internal energy dynamics, deriving quasi-ergodic requirements that must hold for any stationary process due to conservation of energy. Since these requirements are formulated in terms of observable quantities, they can be used to explicitly identify the timescale where valid transport coefficients can be obtained. This result is significant because it provides a straightforward way to homogenize the dynamics of multiphase flow in porous media

which does not obey equipartition of energy, particularly with slow fluctuations.
We apply our theory to derive transport coefficients for immiscible fluid flow through porous media, demonstrating that pressure fluctuations observed in experiments can be non-Gaussian due to co-operative effects that are caused by capillary events. We show that the macroscopic dynamics can still be homogenized if the timescale for averaging is chosen such that these fluctuations perform no net work on the system. We further demonstrate that changes to fluid topology are responsible for non-ergodic effects, and that time-and-space averages provide a natural mechanism to account for discrete changes based on the topological residence time associated with a particular micro-state of the system.
Following that methodology, we derive Darcy's law for single phase flow and the 2-phase Darcy equations for multiphase flow at stationary ("steady-state") conditions. The equations have the same form as the 2-phase Darcy equation introduced as a phenomenological extension to Darcy' s law. Cross terms in relative permeability arise from having experimental access to phase pressures independently.

Participation:

In-Person

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Poster / 263

DoE-based history matching for probabilistic integrity analysis – a case study of the FE-experiment at Mt. Terri

Author: Jörg Buchwald[1]

Co-authors: Sonja Kaiser [2]; Wenqing Wang [1]; Olaf Kolditz [1]; Thomas Nagel [2]

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For the performance assessment of nuclear waste repositories, a thorough analysis of the uncertainty and sensitivity of the underlying processes is necessary. Whereas a detailed experimental investigation of the final repository site is infeasible due to numerous reasons, the verification and validation of the numerical tools under realistic conditions using experimental data of underground research laboratories are all the more important.
One of such experiment is the FE-experiment at the URL site in Mt. Terri - a full-scale multiple heater test in the Opalinus clay in Switzerland which simulates "as realistically as possible, the construction, waste emplacement, backfilling and early post-closure evolution of a spent fuel/vitrified high-level waste disposal tunnel according to the Swiss repository concept." [H. Müller et al. 2017]
In our contribution, we present an application of design-of-experiment-based history matching as an approach to reduce and investigate parameter uncertainties in finite-element models for repositories of high-level radioactive waste [Buchwald 2020]. We combine experimental data from the FE-experiment at the Mt. Terri site in Switzerland with thermo-hydro-mechanical modeling using the open-source package OpenGeoSys. The parameter space was reduced by an initial parameter screening to find heavy hitters and an experiment-matching procedure using Monte-Carlo sampling on a Gaussian proxy model to fit modeling responses. The resulting parameter bounds were used in a subsequent uncertainty quantification and global sensitivity analysis based on the proxy model demonstrating the impact of parameter sensitivities.

Participation:

In-Person

References:

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Buchwald, J., Chaudhry, A. A., Yoshioka, K., Kolditz, O., Attinger, S., & Nagel, T. (2020). DoE-based history matching for probabilistic uncertainty quantification of thermo-hydro-mechanical processes around heat sources in clay rocks. International Journal of Rock Mechanics and Mining Sciences, 134, 104481.

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MS01 / 264

Geochemical reactions of iron oxides with hydrogen in the porespace of sandstones: Processes, kinetics & limitations of the extent of reaction.

Author: Christian Ostertag-Henning[1]

[1] *Federal Institute for Geosciences and Natural Resources*

Corresponding Author: christian.ostertag-henning@bgr.de

Over the last years the interest in molecular hydrogen (H2) has soared: in many countries an accelarating energy transition is considering hydrogen as the main energy carrier of the future. To enable large scale storage for hydrogen, research on subsurface storage options in geologic structures as artificially created caverns in evaporites (e.g. salt domes) or depleted gas fields mainly in

sandstones is pivotal. Some countries as Germany have large volumes available in existing and additionally mineable caverns being the preferred option, but many regions in Europe will continue to use porous rocks –and there mainly sandstone reservoirs of depleted natural gas fields –as underground storage option. In these sandstones geochemical reactions of the molecular hydrogen with dissolved ions in the pore water –and foremost –on reactive mineral surfaces have to be considered in risc assessments for selecting the most suitable rock formations. Some minerals may oxidize hydrogen resulting in a loss of hydrogen and the production of either water or hydrogen sulfide. These products may enhance the alteration of the rock by increasing dissolution-precipitation reactions – or impart on the recoverable gas quality e.g. by traces of hydrogen sulfide (Heinemann et al. 2021). In this contribution the results from geochemical experiments at in situ conditions (elevated pressures and temperatures as in the subsurface in presenc of a liquid water phase) of one common reactive mineral in many sandstones –the iron oxide hematite Fe2O3 –will be presented. The discussion will focus on details on the processes observed, the kinetics of the overall oxidation of hydrogen by hematite, and parameters limiting the extent of the oxidation of hydrogen. An interesting link to ongoing research results in photo(catalytic) water splitting on hematite surfaces has emerged during the study. In addition, for a set of five different natural sandstone samples from the Bunter formation with different contents ot hematite the extent of the reaction was investigated over one month at a pressure of 120 bars and a temperature of 120℃. The overall oxidation of hydrogen was low, but significant differences were apperent between the rocks. Spatially resolved analyses by optical microscopy and Raman spectroscopy allowed to document the reaction products in the intact pore space in the sandstones during and after experiments, pointing to mineral matrix effects on geochemical reactions and hence changes in porosity, pore throat diameters and permeability. These findings will help in delineating guidelines for selecting the formations best suitable for storing hydrogen for extended times in subsurface sandstone reservoirs.

Participation:

In-Person

References:

Heinemann et al. (2021): Enabling large-scale hydrogen storage in porous media –the scientific challenges. –Energy Environ. Sci., 2021,14, 853-864.

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Poster / 265

Numerical design of nano-porous carbon binder domain (CBD) phase in lithium-ion battery electrodes

Author: Ruihuan Ge[None]

Co-authors: Denis Cumming [1]; Rachel Smith

[1] *The University of Sheffield*

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Lithium-ion battery performance can be significantly affected by porous electrode microstructures. The carbon binder domain (CBD) within an electrode structure is used to enhance mechanical stability and facilitate electronic conduction. The understanding of the CBD phase microstructure and how it affects the complex coupled transport processes is crucial. Inspired by the bimodal pore size distribution of electrode structures, a random field method is proposed to generate the multiple phase porous electrode structures in this work. Using this approach, the nano-porous CBD phase with tuneable pore size and transport properties can be generated. The effect of CBD phase distributions on the battery performance is evaluated. It is found that the increased nano-porosity from 0.3-0.6 can increase specific capacity of battery electrodes by 50 to 100%. For the first time, the nano-porous CBD phase and corresponding properties can be manipulated by algorithms - this gives new insights on the battery electrode design.

Participation:

In-Person

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Poster / 266

Microfluidic study of hydrogen conversion by Archea in porous media. A pore-scale investigation of gas conversion and controlling parameters under dynamic conditions.

Authors: Patrick Jasek[None]; Holger Ott[1]

Co-authors: Hannes Konegger ; Saeid Sadeghnejad ; Loibner Andreas ; Frieder Enzmann

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The necessity to scale energy storage capacities in Europe is vital for expanding renewable energy production and avoiding shortcomings in energy supply. In decarbonizing energy systems, hydrogen, in its diverse colors, will play a crucial role as an energy carrier. Storing hydrogen in the subsurface comes with various uncertainties. Independent investigations of underground hydrogen storage revealed that hydrogen is utilized as substrate by Archean cultures in the reservoir leading to environment-controlled reactions.

This study investigates site-extracted and brine-suspended cultures in a microfluidic setup. Biomass accumulation in pore space under saturated and anaerobic flow conditions has shown that bacteria significantly change the hydraulic properties of porous media, altering both porosity and permeability. Using time-lapse imaging, different modes of bacterial accumulation and preferential channel formation could be observed as a function of the injection velocity. The extracted time series was used in numerical Stokes–Brinkmann flow simulations to estimate intrinsic biomass permeability, velocities, and stresses. The simulation results were validated with experimental data and revealed an average intra-biomass permeability of 100±30 mD.
Further analyses concerning the advective nutrient supply potential were conducted to estimate the controlling parameters like the Peclet number. The selected velocity impacts the average biomass cluster size and, herewith, also, the nutrient distribution within the biomass. Furthermore, biomass activity in the presence of a nutrient gas blend of carbon dioxide and hydrogen was investigated in a dynamic flow experiment at elevated pressure and temperature.
The novel setup allowed us to continuously monitor biomass growth, related system responses, and compositional gas changes. Conclusively, an advective nutrient supply in biomass is considered more efficient than a purely diffusive one and might lead to higher metabolic activity and substrate conversion rates, which is particularly interesting for engineered subsurface applications.

Participation:

In-Person

References:

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MS12 / 267

Polytopal Discontinuos Galerkin discretization of the fully-coupled thermo-poroelastic problem

Author: Michele Botti[1]

Co-authors: Paola Francesca Antonietti [1]; Stefano Bonetti [1]

[1] *Politecnico di Milano*

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Poroelasticity inspects the interaction among fluid flow and elastic deformations within a porous material. In several applications in the context of environmental sustainability, such as geothermal energy production and CO2 sequestration, temperature plays an important role in the description of the physical phenomena. Therefore, in order to correctly describe these geological processes, the differential problem should also take into account the influence of the temperature, leading to a fully-coupled thermo-poroelastic system of equations.

We present and analyze an arbitrary-order Discontinuous Galerkin method for the numerical modelling of the non-linear thermo-poroelastic problem based on a novel four-field weak formulation.

The proposed method is designed to support general polygonal and polyhedral elements. This is a key feature in geological modeling in order to handle fractures and degenerate elements arising in the case of compaction or erosion. To handle the non-linear convective transport term in the energy conservation equation we adopt a fixed-point linearization strategy and different linearizations are examined.

We perform a robust stability analysis for the linearized semi-discrete problem under mild requirements on the problem data. A priori hp-version error estimates in suitable energy norms are also derived. A complete set of numerical simulations is presented in order to validate the theoretical analysis, to inspect numerically the robustness properties, and to test the capability of the proposed method in a practical scenario inspired by a geothermal problem.

Participation:

In-Person

References:

- P..F. Antonietti, S. Bonetti, M. Botti, Discontinuous Galerkin approximation of the fully-coupled thermo-poroelastic problem, SIAM J. Sci. Comput., 2022, in press [arXiv:2205.04262]

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268

Utilizing Multi-scale Computed Tomography to Understand Pore Structures of Carbonate Rich Samples for Geologic Carbon Sequestration in the Southeastern, US.

Author: Otis Williams[1]

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Geologic Carbon Sequestration (GCS) is a promising technology that can be utilized to lower atmospheric CO2 emissions. In these systems, atmospheric CO2 is captured and injected into a deep saline aquifer for permanent storage. Once injected, CO2 interacts with the formation brine and existing minerals which can lead to permanent mineral trapping of the CO2. One major challenge of GCS is evaluating the timescale and extent to which CO2 will be transformed into the desired carbonate minerals. Previous work has shown that this timescale is highly dependent on the geologic formation's characteristics where sandstones and carbonates may be promising storage formations. Carbonate minerals react quickly with the CO2–brine mixture, but the benefit or drawback of this is yet to be fully established. The rate, extent, and impact of reactions of formation properties are difficult to predict in part due to the complex, multi-scale nature of the pore structure of carbonate formations. Using a multi-scale method of 3D X-ray micro computed tomography (CT) imaging, the pore structure of potential carbonate storage formations is examined on varying scales. Images

are processed to discern multi-scale porosity, pore connectivity, and the accessible surface area of reactive mineral phases. Data for formations with varying mineralogy are then compared.

Participation:

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References:

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MS01 / **269**

Gas trapping dynamics in heterogeneous sandstones imaged using synchrotron time-lapse tomography.

Authors: Catrin Harris[1]; Senyou An[2]; Vincenzo Cunsolo[3]; Samuel Jackson[4]; Ann Muggeridge[3]; Sam Krevor[None]

[1] *Student*

[2] *University of Manchester, Imperial College London*

[3] *Imperial College London*

[4] *CSIRO*

Corresponding Authors: s.krevor@imperial.ac.uk, v.cunsolo@imperial.ac.uk, ch2919@ic.ac.uk, s.an@imperial.ac.uk, samuel.jackson@csiro.au, a.muggeridge@imperial.ac.uk

Geological heterogeneities impact the timescale and distribution of capillary trapping of CO_2 in aquifers [1,2]. Natural capillary pressure barriers trap the non-wetting phase at saturations greater than expected from pore-scale residual trapping processes alone, potentially providing greater CO_2 storage capacity. Capillary heterogeneity trapping has the potential to significantly improve the security of CO_2 storage in underground aquifers by immobilizing a large proportion of the injected CO_2 [1,2], however the connection between pore-scale fluid dynamics and larger scale flow processes have yet to be properly elucidated. The dynamics of the flow through pore throats may play a significant role in geological carbon storage [3,4], particularly at the boundary between different grain sizes. However, it is heterogeneity at centimetre-scale, over many thousands of pores, that leads to the larger scale phenomena of capillary heterogeneity trapping.

In this experimental campaign, state of the art synchrotron-based X-ray micro-CT experiments at the European Synchrotron (ESRF) were performed to investigate pore-scale flow dynamics in heterogenous sandstone cores over centimetre-scale fields of view. To investigate the impact of mm-cm scale natural geological heterogeneities on fluid migration and trapping, we performed experiments on 3 different sandstone samples: Bentheimer with layers perpendicular to flow, Bentheimer with layers parallel to flow and Bunter sandstone from a UK target storage site, the Endurance field. To evaluate the rate dependency of trapping, experiments over 2 different rates were compared to explore potential trapping within a range of carbon sequestration projects.

The high energy of the ID19 beamline at ESRF allowed us to capture frontal advance and trapping dynamics at pore-scale resolution (6.5 μm) in large heterogeneous consolidated samples (6 cm). With time resolution of 3 minutes, we observed unsteady state displacements, the prevailing conditions at most storage sites [1,4]. We captured dynamically both drainage and subsequent imbibition, proceeding until the residual saturation was reached. Pore-scale trapping mechanisms were captured with a field of view over the continuum core-scale, allowing us to investigate how larger scale capillary heterogeneity trapping processes are impacted by pore-scale events. Such experimental observations resolving trapping over many pores, representative of the large-scale process, are crucial for model validation, development and ultimately storage predictions [5].

We were able to observe, at the pore-scale, the transient interaction of the fluids with different types of layered heterogeneity. The heterogeneity impacted pore-filling events, and subsequent imbibition, allowing us to quantify the path to residual trapping. Consistent with numerical simulations [2], injection rate impacted capillary trapping with lower capillary number resulting in a greater amount of capillary heterogeneity trapping. The results from this synchrotron campaign advance our understanding of the impact of heterogeneity on the dynamics of capillary trapping within CO_2 storage sites.

Participation:

In-Person

References:

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[5] Jackson, S. J., & Krevor, S. (2020). Small-scale capillary heterogeneity linked to rapid plume migration during CO2 storage. Geophysical Research Letters, 47. https://doi.org/10.1029/2020GL088616

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Superposition of colloid-surface repulsion and incomplete pore scale mixing explains emergence of fast-and slow-attaching subpopulations from identical individuals, and depletion of fast-attachers

with increasing transport distance under unfavorable conditions

Authors: William Johnson[1]; Santiago Jurado[1]

[1] *University of Utah Department of Geology & Geophysics*

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Colloid transport in porous media is notoriously unpredictable under unfavorable attachment conditions, wherein nanoscale repulsion exists between colloids and surfaces, e.g., environmental systems, or any system in which colloid and porous media surfaces carry like charges (i.e., both surfaces negative or both surfaces positive). Repulsion impacts colloid transport at the pore-scale by driving larger (and longer) near-surface transport distances (and times), across surfaces prior to attachment. At the continuum-scale (e.g., column or field scale), the distribution of colloids downgradient from their source is exponential under favorable conditions and non-exponential under unfavorable conditions. Explaining/predicting these continuum-scale distributions from source under unfavorable conditions can be accomplished under two assumptions: a) that fast- and slow-attaching colloid subpopulations emerge from an overall population of identical individuals; and b) that the fast-attaching subpopulation is depleted with increased transport distance. This paper confirms the emergence of fast and slow attaching sub-populations from an overall population of identical individuals in pore network experiments. We demonstrate in experiments and mechanistic trajectory simulations the mechanisms underlying this differentiation, which result from the combined impacts of repulsion and flow field topology. Fast-attaching colloids were predominantly delivered proximal to forward flow stagnation point (FFSP) where fluid streamlines impinge on grain surfaces on the upstream sides of grains, allowing fast attachment in this low-shear region. In contrast, slow-attaching colloids intercepted the near surface fluid predominantly at locations lateral to FFSP. At the pore network scale, colloid residence times in near-surface fluid upgradient of the grain to which the given colloid attached were far lower for fast-attaching colloids relative to slow-attaching colloids. Fast-attaching colloid trajectories existed predominantly on streamlines in the bulk fluid prior to intercepting the grain onto which they attached. In contrast, slow-attaching colloid trajectories intercepted near-surface fluid associated with multiple grains prior to intercepting the grain onto which they attached. The existence of narrow zones of incomplete pore-scale mixing (lamellae) that extend from the rear flow stagnation point (RFSP) on the downstream sides of grains and often extend to FFSP of downgradient grains to form grain-connecting lamellae (GCL) suggest that slow-attaching colloids move predominantly along the GCL network. Persistence of FFSP and GCL networks with downgradient distance is posited to drive depletion of fast-attaching colloids in the FFSP network and drive accumulation of slow-attaching colloids in the GCL network. The combined experiments and simulations explain why fast- and slow-attaching subpopulations arise from identical colloids and suggest a mechanism for preferential depletion of the fast-attaching subpopulation with downgradient transport. Figure 1: Inlet zone of 2-D porous medium. Upper panel: Binary image of lamellae superimposed across time during fluorescent tracer invasion. Blue and red circles represent colloid near-surface entry locations for fast and slow attachers under unfavorable conditions. Arrows indicate numbers of colloids delivered to grains (pillars), with asterisks denoting non-FFSP locations. Green dashed lines denote GCL not captured in binarized image. Bottom panel: Cumulative frequencies of colloid near surface entry as a function of angular distance from FFSP for favorable (bottom left) and unfavorable (bottom right) conditions.

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MS08 / **271**

Mixing in Porous Media: Observations and Modeling of the Local Concentration PDF

Authors: Guillem Sole-Mari[1]; Saif Farhat[2]; Joris Heyman[3]; Diogo Bolster[4]; Daniel Hallack[2]; Tanguy Le Borgne[5]

[1] *Université de Rennes 1*

[2] *University of Notre Dame*

[3] *CNRS*

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In most types of natural and artificial porous media, even before taking larger-scale (e.g., permeability) heterogeneities into consideration, fluid flow usually exhibits complex random local velocity patterns. This has traditionally made scalar transport difficult to accurately predict whenever pore-scale concentration variability is of concern, which is usually the case when dealing with nonlinear processes such as chemical reactions, especially at high Péclet numbers.
This problem can be approached by representing the microscale concentration variability as a probability density function (PDF). Concentration probability density is then transported (i) spatially through macroscopic advection-dispersion and (ii) over the "concentration space"due to local mixing.
For instance, a classical model for the local mixing term, Interaction by Exchange with the Mean (IEM), has the form of a probability density drift (advection) towards the local mean concentration. This model is based on strong assumptions and generally fails to reproduce observations. A recently proposed multirate IEM model (MRIEM) attempts to overcome the simplicity of the former by allowing multiple simultaneous rates of drift towards the mean, but still lacks a direct link to the structure of the porous medium or the actual physics of the local mixing process.
In this work we further investigate the mathematical nature of the local mixing term and develop an improved model based on microscale physics and heterogeneity statistics, producing results that agree with recent observations from direct numerical simulations.

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In-Person

References:

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Energy Transition Focused Abstracts:

Poster / **273**

Acceleration of Optimal Bayesian Experimental Design via Decision Trees Methods with Orthgonality Constraint

Authors: Alexander Tarakanov[1]; Grigorii Buklei[1]

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Optimal Bayesian Experimental Design is one of the methods for data acquisition system optimization that is frequently utilized in subsurface flow problems. In this method utility function that measures expected quality of the experiment is derived from the first principles of probability and statistics as a function of design parameters (aka sensor location). Therefore, the optimal experimental scheme can be found as a maximum of that utility function.

The most significant advantage of this method is solid Mathematical foundations.
Unfortunately, direct calculation of the Utility Function is computationally expensive, because it requires nested MCMC integration [1].

In the author's previous work [2] it was shown that Polynomial Chaos Expansion (PCE) can be utilized to accelerate Bayesian Experimental Design significantly. Basically, a novel approach for the utilization of PCE to avoid nested MCMC integration was proposed. The key idea for developing of that novel technique was the orthogonality of basis polynomial functions in PCE.

Despite the advantages of PCE, Decsiion Trees and Gradient Boosting methods seems to be an attractive altermative to PCE due to high popularity and simplicity in tuning. Therefore, the present work shows how orthogonality ideas can be extended to Decision Trees or Gradient Boosting like methods to provide acceleration of Bayesian Experimental Design. In other words, the novel algorithm for construction of the Gradient Boosted trees with specific orthogonality constraint was developed and examined on several test cases that include flow in porous media. Additionally, validation against classical methods is provided.

Participation:

In-Person

References:

[1]Xun Huan, Youssef M. Marzouk, Simulation-based optimal Bayesian experimental design for nonlinear systems, Journal of Computational Physics, Volume 232, Issue 1, 2013, Pages 288-317, ISSN 0021-9991, https://doi.org/10.1016/j.jcp.2012.08.013.

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MS11 / 274

Experimental observation of microbial growth using a microfluidics approach

Author: Christian Truitt Lüddeke[1]

Co-authors: Birger Hagemann [1]; Leonhard Ganzer [1]; Gion Joel Strobel [1]

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For a successful transition towards renewable energy resources, hydrogen is playing an increasingly significant role. In order to have a sufficient amount of hydrogen available to meet the demand, it has to be stored in suitable facilities. The storage of hydrogen in subsurface porous media is considered to be a viable option. The most promising sites are currently used as underground gas storages. Natural gas usually contains a certain amount of CO2 which can remain in the porous media and methanogenic archaea tend to be present in the remaining residual water. This poses challenges to a potential underground hydrogen storage. When the microbes come into contact with a gaseous H2-CO2 mixture they consume it, resulting in the production of CH4 and water according to Sabatier (1913). In this study, the microbial behavior and the measurement of produced gases is experimentally examined and observed.

The experimental setup consists of two inline pressure sensors, two syringes, one micromodel representing a uniform porous structure with a porosity of 28 % and a permeability of 10 D, a micromodelholder, a microscope and a micro gas chromatograph (micro GC). A liquid mixture of culture media and methanogens (in this experiment methanotermococcus thermolithotrophicus) is prepared in a Hamilton 10ml glass syringe and injected into the micromodel which has been placed under the objective of the microscope equipped with various magnification lenses and a high-precision camera. The microchip is heated up to a temperature of 65℃, which is considered to be optimal for the growth of this type of archaea. Simultaneously, two Hamilton 8ml steel syringes are filled with a gaseous mixture of 80% H2 and 20% CO2. When the micromodel is completely saturated with the media-microbes-mixture, the H2-CO2 mixture is injected into the microchip, resulting in a two-phase saturation. The objective of the microscope is positioned at selected locations on the microchip near a gas-liquid interface. Over time, images with a transmitted light and reflected fluorescence light at a 40-time magnification are taken. The analysis of the images is conducted with the MATLAB image processing tool box.

The results of the image processing show that in the presence of hydrogen and carbon dioxide, the number of microbes grow with time. Initially, the microbes tend to be in a lag phase which lasts for a few hours. After this phase, they start to grow and their number increases. After converting nearly all of the gas, the microbes stop growing. Produced methane has been detected by the micro GC. In general, the stated experimental procedure provides the opportunity to examine the microbial behavior under the influence of hydrogen and carbon dioxide on a pore scale.

Participation:

In-Person

References:

Sabatier, Paul (1913): La Catalyse en Chimie Organique. Paris: Librairie Polytechnique

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Energy Transition Focused Abstracts:

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A Pore-Level Multiscale Method for the Elastic Deformation of Fractured Porous Media

Author: Kangan Li[1]

Co-author: Yashar Mehmani [1]

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In direct numerical simulations (DNS) of mechanical deformation of fractured porous media, the momentum equation is discretized and solved with a fine-grid solver (e.g., finite elements) on a 3D image (e.g., X-ray μCT). While this yields a high-fidelity solution, DNS is computationally expensive. In this work, we present a pore-level multiscale method (PLMM) that approximates DNS efficiently and with controllable accuracy to model the linear elastic response of porous solids with arbitrary microstructures and crack patterns. PLMM decomposes the solid into subdomains, over which local basis and correction functions are built. These functions are coupled with a global problem to yield an approximate solution, whose errors can be iteratively corrected. A key novelty of our PLMM is that the decomposition need not conform to the cracks, unlike a previous variant developed by the authors. This paves the way towards solving crack nucleation and growth problems in the future without having to dynamically update the decomposition. We explore different strategies for capturing cracks through either the basis or correction functions, and we discuss the implications of each on the convergence rate and computational cost.

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Energy Transition Focused Abstracts:

Poster / 276

Wind erosion suppression using biological methods revisited: The use of microbial/enzymatic-induced carbonate precipitation and biopolymers

Author: Ehsan Nikooee[1]

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Dust emission induced by wind erosion affects crop production, the aviation industry, and human health, to name a few. Wind-borne dust particles can have several environmental and health implications. They can carry pathogenic microorganisms and thereby pose health threats. Besides, having entered surface water and oceans, they change water chemistry and quality, subsequently affecting the native ecosystem. Dust emissions not only affect the inhabitants of their source of origin but also have detrimental effects on the life quality of the settlements far away. Thus, dust emission is a global environmental challenge.

Over the past few decades, the need to achieve minimum greenhouse gas emissions has led scientists to search for new compounds and techniques for wind erosion suppression. Having encountered naturally cemented sedimentary formations such as Stromatolite in Western Australia, the idea of a bio-mediated or bio-inspired technique for soil stabilization has appealed to several studies. Therefore, there have been recently numerous studies on the use of biological methods such as microbial carbonate precipitation (MICP) [1-3], enzymatic carbonate precipitation [4-7], and biopolymers for wind erosion mitigation [8].

In this contribution, we briefly introduce these methods, and their main stabilization mechanisms, such as the involved biogeochemical reactions, types of microorganisms, and the induced mechanical effects. Care has been taken to highlight the merits and demerits of each approach and elucidate the challenges in their field-scale applications. Finally, future research perspectives and directions are introduced.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS09 / **277**

Image-based pore-scale simulations of nuclear magnetic resonance response for enhanced reservoir characterization

Author: Matheus Ribeiro[1]

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Nuclear Magnetic Resonance (NMR) is a powerful tool to assess physical quantities that characterize porous media, offering detailed information about the fluid molecules confined in the pore space. This work presents a computational implementation of image-based simulations of NMR experiments in porous media using the Random Walk method with a particular focus on reservoir rocks. We explore and discuss the computational challenges of running such simulations on personal hardware instead of using multicore clusters, which is the conventional approach. In that sense, the proposed solution includes a scheme for data compression and a strategy for massive parallelization in the graphics processing unit. Moreover, we present applications simulating NMR diffusometry and relaxometry experiments. In the first study, the time-dependent apparent diffusion coefficient is measured by simulating the Pulsed-Field Gradient NMR technique. This quantity's asymptotic behavior in both short and long-time ranges is then used to recover the surface-to-volume ratio and the tortuosity of the underlying porous medium. We explore the correlation between the recovered parameters and the absolute permeability in a set of synthetic granular media and segmented microtomographic images of sandstones and carbonates. In the second study, we explore the influence of the diffusive relaxation mechanism in the transverse relaxation time, T_2. The relevance of this mechanism arises in the presence of strong internal magnetic field gradients induced by a pronounced contrast between the magnetic susceptibility of fluid molecules and mineral components of the solid phase. These simulations require a two-step workflow: in the first step, we compute a spatial description of the magnetic field inside the pore space by solving Maxwell equations under zero-current condition using an image-based finite elements implementation; second, we feed our random walk simulations with the computed field map, incorporating its dynamic effect in the magnetized spins. We perform such simulations in sintered models of glass beads containing localized concentrations of iron oxides and sandstones of varying mineral compositions. Not only will this enhanced relaxation alter the otherwise straightforward interpretation of T_2 relaxation times into pore sizes, but it may also indicate the presence of clay components in the mineral phase. In both studies, experimental data is provided for comparison purposes.

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Energy Transition Focused Abstracts:

MS04 / 278

Linear stability analysis for the formation of wrinkles on confined swelling hydrogels

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Wrinkling, buckling and creasing instabilities are some of the most familiar phenomena observed in the study of soft materials including hydrogels. They arise when there is mechanical confinement, for example from a fixed base or from hoop stresses in swelling spheres, leading to the preferential formation of wrinkles to relieve shear stresses from the confining strain. These have long been studied as purely elastic instabilities, with a mechanism akin to Biot's classic stability analysis of an elastic half-space under pre-stress. Here, we argue that the swelling process itself is a key part of the mechanism driving these instabilities by carrying out a linear stability analysis of the swelling of a finite layer of gel under horizontal confinement. This stability analysis uses our own linear-elastic-nonlinear-swelling theory for hydrogels that captures the nonlinearities arising from the large isotropic strains when a gel takes on water but allows for an analytically tractable approach through linearising around small deviatoric strains. Under this theory, the physical processes driving the swelling and drying that forms the wrinkles can be easily seen, unlike in fully nonlinear approaches where only a condition for marginal stability can be derived through minimisation of free energy. Furthermore, the growth rate of a given instability is deduced, allowing us to determine the separate influences of wavenumber, layer thickness and material properties on the stability of the water-gel interface. It is observed that the anchoring effect of the fixed base of the gel layer stabilises low-wavenumber (long-wavelength) wrinkles, whilst the growth rate increases unboundedly with the wavenumber, leading to an 'ultraviolet catastrophe'whereby infinitesimally small wavenumbers grow at an infinite rate. We propose solving this by introducing a surface tension at the gel-water interface that serves to stabilise short-wavelength instabilities. The effect of this surface tension is quantified for two different mechanisms; firstly, a surface tension that arises as a bulk elastic discontinuity in stress, and secondly as one arising from a discontinuity in the pore pressure of water between the liquid and gel phases. Quantitative differences between these two mechanisms are discussed, and the evolution of the most unstable wavenumber in time is evaluated and compared to the smoothing and healing of these instabilities seen in experiments, where wrinkles are known to coarsen and, in some cases, disappear entirely as the gel layer imbibes more water. We show that our theory, with the addition of surface tension, can describe all these observations and postulate how further experimentation could determine the true physical origin of the surface tension at the interface.

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Energy Transition Focused Abstracts:

MS01 / 280

Salinity gradients and salt precipitation due to hydrogen injection in saline aquifers and reservoirs

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Co-authors: Mostafa Borji [1]; Zaid Jangda [2]; Kamaljit Singh [2]; Hannah Menke [2]; Ben Callow ; Shan Wang ; Sharon Ellman [3]; Veerle Cnudde [4]; Hannelore Derluyn [5]; Tom Bultreys [1]

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As a strategy to match renewable energy supply and demand, surplus energy can be converted into hydrogen gas and stored in the pore space of geological subsurface formations such as saline aquifers and depleted gas reservoirs. Although similar operations with natural gas and CO2 are well studied, H2 has unique chemical and physical properties which, combined with cyclic injection and withdrawal, may cause complex phenomena that affect the efficiency and safety of storage operations. In this study, we investigate the risk of H2 injectivity impairment due to salt precipitation in the pores, driven by the interplay between the evaporation of water from the brine (originally present in the reservoir) into the injected gas, salt diffusion, and capillary fluid flow. To do so, we investigate the pore-scale salt concentration distribution and resulting precipitation patterns during gas injection in sandstone using micro-CT imaging. We present the first of such dry-out experiments performed with hydrogen gas under reservoir pressure and temperature, supplemented with N2 experiments to evaluate the influence of the original salt concentration and flow rate on the salinity gradient during drying, as well as on the resulting salt precipitation. In order to explain and predict the associated permeability impairment, we set up a pore network model with pore structure modification due to precipitated salt in individual pores, measured during the experiment. Our experimental results indicate that salt precipitation can cause up to a 30% reduction in permeability, which was also supported by numerical model outputs. The results of this study provide useful information on the impact of salt precipitation, and other geochemical and microbiological effects driven by concentration gradients on storage efficiency.

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MS20 / 281

Theoretical and experimental study of intracellular transport using a porous media approach

Author: Olivier Destrian[1]

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Intracellular transport of macromolecules is essential to numerous biological functions, particularly for apoptosis (programmed cell death). During this process, specialised proteins called caspases are produced and transported within the cell. Their activity leads to the reorganisation of cytoplasmic structures, including the actin cytoskeleton. The rearrangement of this fibrous structure may in return alter the intracellular transport properties of caspases (effective diffusivity and reaction rates) and therefore their activity. To our knowledge, the impact of the cytoskeleton remodelling on the intracellular transport properties has remained largely unexplored.

Here we propose to combine porous media theory and cell biology experiments to study the coupling between the reorganisation of the actin cytoskeleton and the intracellular transport of large proteins. At the local scale, the cytoplasm is modelled as a nanometric fibrous porous medium surrounded by a homogeneous fluid. With a radius of 4 nm, the actin fibres typically form structures with a pore size ranging from 10nm to 100nm [2]. The diffusive particles considered have a nanometric radius, leading to significant tortuous and hydrodynamic diffusional hindrances [3]. A homogenisation procedure is carried using the Volume Averaging Method [4], allowing the determination of the relevant effective transport properties and cell scale transport equations. The link between actin structures (local scale) and effective transport properties (cell scale) is investigated by numerically solving closure problems arising from the procedure. Finally, the cell scale model is solved on specific cases for validation against experimental measurements inside living cells. Cytoplasmic diffusion of endogenously expressed fluorescent tracers is studied quantitatively using both Fluorescence Recovery After Photobleaching (FRAP) and Fluorescence Correlation Spectroscopy (FCS) techniques.

This multidisciplinary work may lead to a better understanding of diffusion-reaction processes in biological porous structures, with possible implications on apoptosis related disorders such as autoimmune diseases and cancer.

Participation:

In-Person

References:

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Poster / **282**

Enhancing backfill thermal properties by combining granular phase change materials, graphite and glass

Author: Tairu Chen[None]

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Phase change materials (PCMs) can store and release heat at a relatively constant temperature. Incorporating PCMs into mixtures for backfill materials may improve their thermal energy density and thus contribute to the enhancement of borehole thermal energy storage and shallow geothermal energy systems. However, PCMs might reduce the overall heat transfer between the borehole and the surrounding ground because of their low thermal conductivity. Thus, other additives may be needed to improve the effective thermal conductivity of the backfill-ground system, while maintaining desirable heat capacity and then the corresponding efficiency of the shallow geothermal systems. This study incorporates encapsulated PCMs (EPCMs) and graphite into glass fines with the purpose of using the mixtures as backfill materials. The heat capacity and thermal conductivity of mixtures with different content of each component are measured in the laboratory. In addition, a computed tomography slice, which contains EPCMs, graphite, glass, and air phases, is selected to study the heat transfer at the particle scale. The experimental data agree with the simulated results. The findings in this study can be used in geothermal system design and contribute to the transition from fossil-based energy systems to renewable energy sources.

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MS15 / **283**

Practical Tera-scale 3D Super Resolution Approaching a 1-micron Resolved 1-inch Core Plug

Authors: Ying Da Wang[1]; Kunning Tang[1]; Ryan Armstrong[None]; Peyman Mostaghimi[None]

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The trade-off between the field of view (FOV) and resolution of micro-computed tomography (micro-CT) is a hardware bottleneck limits capturing both heterogeneity and micro-structure detail. Efficient super resolution methods combine the upper limits of both FOV and voxel resolution, while efficient modelling permits analysis of the large domain. A low resolution image of a 1-inch sandstone core plug and an unregistered high resolution (1-micron) sample trains an efficient and world-first 3D un-paired super resolution convolutional neural network, Dual-CycleSR. The resulting 25,000 x 25,000 x 50,000 domain provides unprecedented geometric fidelity over a full-sized core plug and reveals spatial heterogeneity that is captured by pore-to-core upscaling, with which forward-modelling produces a close match with unsteady-state core flooding production curves.

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Poster / 284

Stability assessment of foam enhanced by surfactant, polymer and nanoparticles in the presence of petroleum hydrocarbons

Author: Adil Baigadilov[1]

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The risk of environmental pollution, particularly groundwater contamination, has increased over the last century as a result of the growth of industry. Light non-aqueous phase liquids (LNAPLs) are one of the most common contaminants and refined petroleum hydrocarbons (RPHs-diesel, gasoline, motor oil, etc.) are typical examples [1, 2]. Heterogeneity in the subsurface represents one of the main issues for LNAPLs remediation, conventional pump-and-treat method rarely exceeds 60% of efficiency [3]. However, some studies demonstrating the non-Newtonian shear-thinning behavior

of foam in highly permeable porous media point to the promising potential of foam to improve remediation yields [4, 5].
The use of aqueous foam in environmental remediation (ER) was inspired by enhanced oil recovery (EOR), and it has already proven to be an excellent displacing fluid for in situ remediation of NAPLs [6 –8]. However, contact with petroleum compounds tends to deteriorate the stability of foam significantly and thus it is a challenge for both foam applications [9, 10]. Many researchers are currently focused on strategies to enhance foam employing numerous additives: i.e. co-surfactants [11, 12], polymers [13, 14], and nanoparticles (NPs) [15, 16]. It is worth noting that all of these studies mainly address foam applications in EOR. The main objective of our work is to evaluate experimentally the stability of foam generated with two or more additives in the presence of RPHs, both in bulk and in porous media.
In order to implement the concept, two environmentally friendly surfactants (sodium dodecyl sulfate (SDS) and cocamidopropyl hydroxysultaine (CAHS)) were experimentally investigated for their foaming ability and stability in the presence of diesel oil using the bulk foam screening method. Stability of complex foam formulations including a combination of surfactants, polymers and NPs were then examined. Two one-dimensional columns packed with sand and coupled in series were used to (i) generate a fully developed foam flow, (ii) evaluate foam stability and recovery efficiency of diesel initially at residual saturation. Mass balance and differential pressure were measured during each injection experiment.
The bulk foam study demonstrated an apparent increase in foam stability in the presence of Diesel when complex foaming solutions were used. The mixture of SDS and CAHS (SC) at a ratio of 1:1 could improve 7.5 times the bulk foam stability in contrast to SDS alone. The presence of NPs enhanced the bulk foam stability up to a factor of 2.6 for the SDS alone and 1.2 for the SC. Among the three types of tested environmentally friendly polymers, xanthan gum (XG) showed the best stabilizing properties compared to carboxymethyl cellulose and guar gum, with increased stability by factors of 3.4, 2, and 1.3 times respectively. Concerning the performance of foam in porous media, complex foaming solutions ranked as SC+XG > SC+NPs > SC > SDS.
Further studies are ongoing to explain how the addition of NPs and polymers affects recovery. Nevertheless, advanced foam formulations clearly exhibited promising perspectives to develop an efficient remediation technique for highly permeable soils contaminated by RPHs.

Participation:

In-Person

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Unveiling Coupled Transport and Reactivity Mechanisms in Shale Caprocks with X-ray Computed Tomography

Author: Manju Pharkavi Murugesu[1]

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Reactive transport is fundamental to subsurface processes such as CO2 sequestration [1], CO2 injection for enhanced geothermal systems and unconventional resource recovery [2], nuclear waste isolation for long-term storage [3], and groundwater contaminant transport [4]. Injectants introduce chemical disequilibrium in geological porous media containing in-situ formation fluid and reactive minerals, causing the onset of a series of dissolution and precipitation reactions. The reactions along rock-fluid interfaces have rapid kinetics and significant impact on porosity and permeability; consequently, flow and storage properties of the geological formation rocks. The coupled reactivity and transport mechanisms have variable outcomes in shales containing multi-scale features including fractures, microcracks and matrices.

Most reactive experiments to date are conducted in batch reactors where reactions at different times are captured, but the dynamic flow component is neglected [5]. Fluid flow determines how the reactants are transported to reaction sites. This has been addressed by several studies that utilized X-ray Computed Tomography (CT) to image reactive transport [6, 7, 8]. Formulation and translation of reactive transport models to field scale is still limited by the lack of model calibration with experimentally observed temporal and spatial data. The interplay between reaction and transport mechanisms is also yet to be fully understood, especially for a multiscale mineralogically heterogenous fractured shale. Accordingly, the unique contribution of this study is the tracking and visualization of reaction-induced alterations in matrix, microcracks, and fractures of shale versus time to provide valuable data for modeling of reactive transport in unconventional geological porous media.

We conducted reactive brine injection in a naturally fractured Wolfcamp core sample for a period of two months while imaging using X-ray CT. The fluid injected is synthetic Wolfcamp formation brine reduced to a pH of 2. Hence, this fluid is analogous to formation brine acidified by the dissolution of CO2. The sample is additionally imaged before and after flow experiments using micro-CT and Scanning Electron Microscope (SEM) to obtain information on mineral alterations at finer scale. Helium pulse decay and Inductively Coupled Plasma (ICP) measurements were conducted to track the permeability of the sample and fluid chemistry within the sample, respectively.

Findings from this study show rapid dissolution of carbonate minerals near fracture-matrix interfaces where reactive fluid had ready access. Dissolution created secondary porosity along fractures and enhanced fluid diffusion into matrix pores. Continued dissolution increased pH of fluid and led to precipitation of scales. Reactive flow also mobilized fines from fracture surfaces, exposing new surface for direct contact with fluid. Because fines on fracture surfaces act as asperites that prop fractures open against the continuous overburden pressure, fines mobilization is associated with fracture closure due to confining stress. Migrating fines also temporarily accumulate at narrow fracture constrictions, diverting flow into matrix pores. This aspect traps fluid in undisturbed low-permeability matrix pores thereby reducing the overall flow and storage property of the formation rocks.

This study, therefore, shows the spatial and temporal effect of coupled reactivity and transport mechanisms, through a combination of experimental methods.

Participation:

Online

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Poster / 286

GPSFLOW: A Novel Simulator for Modelling Underground Hydrogen and Gas Mixture Storage in Rough Reservoir

Author: Zuansi Cai[1]

Co-authors: Keni Zhang [2]; Juan Padrino [1]; Chris McClane [3]; Chaobin Guo [4]; Mark Cullen [5]

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Underground hydrogen storage can store grid-scale energy for balancing both short-term and long-term inter-seasonal supply and demand. However, there is no numerical simulator which is dedicated to the design and optimisation of such energy storage technology at grid scale. A novel multiphase simulator, GPSFLOW (**G**eneral **P**urpose **S**ubsurface **Flow** Simulator), has been developed for modelling reservoir-scale hydrogen and gas mixture (e.g., H2-CO2-CH4-N2) storage in deep saline aquifers and depleted gas fields. The simulator is capable of modelling multiple gas mixture storage over a range of temperatures from 20-200 C and pressure up to 1000 bar on multiple parallel computing platforms. The accuracy of GPSFLOW is verified by comparisons against the NIST online thermophysical database and reported lab experiments, as well as benchmarked against an existing model.
This study built on our newly developed modelling capability and conducted scenario analysis to investigate CO2 cushion gas migration pathways and reservoir pressure in Rough according to the CO2 supply chain in the region, existing wells and historical natural gas data. Hydrogen storage analysis was built on the plausible CO2 cushion gas storage scenarios and investigate the impact of hydrogen injection/withdrawal cycle and storage location on the quality of the extracted hydrogen gas.

Participation:

In-Person

References:

Cai, Z., Zhang, K., & Guo, C. (2022). Development of a Novel Simulator for Modelling Underground Hydrogen and Gas Mixture Storage. International Journal of Hydrogen Energy, 47(14), 8929-8942. https://doi.org/10.1016/j.ijhydene.2021.12.224

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MS01 / 289

Engineering ordered porous structure with direct additive-manufacturing approach for solar thermochemical fuel production

Authors: Da Xu[1]; Meng Lin[1]

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Solar-driven thermochemical fuel processing has shown potential for efficient large-scale solar fuel production due to its broadband solar absorption and favorable thermodynamics and kinetics at high operating temperatures. The porous media is one of the crucial components in the fuel production reactor, which directly converts concentrated solar radiation into heat, enhances heat and mass transport, and provides reactive sites for redox reactions. The coupled multiphysical phenomena involved in a typical reactor require an in-depth understanding of optical propagation, heat and mass transfer, as well as thermochemical reactions in a comprehensive manner. Moreover, these transport and reactive phenomena are closely related to the morphology of the porous reactant. Hence, it opens a pathway for optimizing the reactor with tuned porous structures.

In this study, we introduced the 3D-ordered structures, i.e, TPMS structures, whose morphology can be precisely controlled by their well-defined mathematical expressions. By introducing local anisotropy, we aim at achieving uniform solar absorption as well as temperature distributions to minimize the thermal and chemical stresses in the porous structure for a longer lifetime. The designed porous structures were fabricated by an advanced stereolithography-based ceramic 3D printing method. The fabricated structures were then tested in a dedicated environment chamber operating under a high-flux solar simulator at SUSTech. The local temperature and oxygen sensors were used for probing temperature and partial pressure of oxygen along the sample length which was then linked to optical and reaction phenomena via our high-fidelity modeling framework. This study will offer a verified method for optimizing porous structures for performant solar thermochemical fuel generation.

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290

Effect of elevated pressure and temperature on seepage characteristics of mixed wettability porous media

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Wettability is one of the critical factors affecting fluid distribution and fluid repulsion efficiency within sandstones, and its accurate characterization is crucial for improving gas reservoir recovery. The variation pattern of wettability of rock mineral composition in sandstone reservoirs under high temperatures and high-pressure conditions in deep strata is still unclear. In this paper, we combine molecular dynamics simulation and phase field method to study the variation law of wettability of different minerals under high temperature and high-pressure conditions and carry out a micro-visualization simulation of percolation in mixed wettability porous media. The results show that the wettability of minerals in sandstone is mostly water-wet, and organic matter is non-wetting; the temperature and pressure of the formation have a particular influence on the wettability of minerals, among which the temperature condition has a more significant influence, and the wettability angle of quartz surface decreases from 32 degrees to 10 degrees from 25℃ to 150℃; the residual saturation of gas phase is positively correlated with the content of organic matter, and the breakthrough time of water phase is negatively correlated with the change of residual saturation of gas phase.

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Energy Transition Focused Abstracts:

MS10 / 291

A digital core reconstruction method based on discrete element method considering the actual shape of rock particles

Authors: Chunqi Wang[1]; Jun Yao[1]

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Abstract

Digital core reconstruction is essential for the numerical simulation of reservoir fluid microscopic flow. However, the existing reconstruction methods, including physical experiments and numerical simulation, cannot construct the digital core reflecting the effect of in-situ stresses. The discrete element method (DEM) is considered reliable in solving this problem. However, in the existing studies on digital core construction based on DEM, commonly used disk or spherical particles, the pore shape of reconstructed digital cores cannot reflect the pore shape of natural rock. Therefore, a digital core reconstruction method based on DEM considering the actual shape of particles is proposed in this paper. Firstly, the Gaussian filter was used to preprocess the CT scan images obtained from the ground condition scanning, the improved watershed algorithm was used to segment the rock particles and porous, and the level set method was used to identify the contour of the particles. Then, clumps composed of multiple particles are used in PFC2D to fill the actual particle contour and construct the clump template library. Finally, according to rocks'particle size distribution and porosity, particles are randomly selected from the established clump template library to accumulate and reconstruct the digital core. The proposed method is used to reconstruct the digital cores of three types of sandstones. The results show that the reconstructed digital cores can keep the properties of the actual rock cores well. This study will provide a reference for reconstructing digital cores in deep

(or stress-sensitive) reservoirs.
Keywords: digital core reconstruction; discrete element method; image processing; watershed method; level set method.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS06-B / **293**

Transport of hydrophobic nanoparticles in partially saturated porous media: Attachment at fluid interfaces

Authors: Youssra Rahham[1]; Stephen Dauphinais[1]; Jeffrey Gostick[1]; Marios Ioannidis[1]

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Sub-micron size plastic particles represent a threat to aquatic environments. These colloidal particles are generally hydrophobic and therefore have the potential to attach and accumulate at air-water interfaces. The role of fluid-fluid interfaces as particle collectors has been recognized, but predictive models of nano-colloid transport in partially saturated porous media are still lacking. Such models are valuable in upscaling the interaction of nanoparticles with fluid interfaces in porous media, which arises also in cases of nanoparticle injection for subsurface remediation or oil recovery. Model validation requires the availability of a model colloidal system, one for which the surface forces governing particle-interface interactions are well quantified.

We report here on the use of ethyl cellulose (EC) nanoparticles as a well-characterized surrogate for hydrophobic nano-colloids in porous media. These particles adsorb irreversibly at the air-water and alkane-water interfaces forming dense monolayers. The dynamics of their attachment has been found to be diffusion-controlled at early stages and kinetically controlled otherwise. We develop a Eulerian pore network model (PNM) built using the open-source software, OpenPNM. Simulations are performed on a pore network extracted from a column packed with spherical beads and used to investigate the irreversible adsorption of nanoparticles on trapped immobile non-wetting phase ganglia present in partially saturated porous media. Additionally, we use a continuum description of the transport and interfacial retention processes to interpret pore network modeling results. This upscaled model accounts for advection, dispersion and irreversible retention on fluid-fluid interfaces using a random sequential adsorption framework. This framework introduces a blocking function the parameters of which are independently determined. Scaling of the continuum model reveals that the continuum model response is governed by three dimensionless numbers, namely the Péclet Number (Pe), the Damköhler number (Da), and a dimensionless number (area ratio, A_r) reflecting the adsorption capacity of fluid interfaces relative to the availability of adsorbing particles. The

continuum model was fitted to the PNM results by optimizing three parameters: the dispersion coefficient D_h, the specific interfacial area a_0, and the adsorption constant k_i. The PNM results showed that the attachment of nanoparticles on fluid interfaces increases by decreasing the adsorption barrier and increasing the non-wetting phase saturation (S_{nwp}), which is directly proportional to the interfacial area available for adsorption. The breakthrough curves were compared to a conservative tracer and showed reduced deposition (blocking) and/or unlimited irreversible deposition in case of lower initial nanoparticle concentration. Upscaling resulted in considerable difference between the pore network and the continuum-scale parameters as regards a_0 and k_i, while D_h increased with increasing S_{nwp}. Slow flow regions resulted in dynamics not captured by the continuum model, in the presence of high S_{nwp}. It was also found that adsorption parameters cannot be inferred from effluent data when A_r >10.

These findings provide valuable insights into the behavior of nanoparticles in partially saturated porous media, and their particular interactions with fluid-fluid interfaces. This research contributes to the understanding of nanoplastics transport in aquifers for risk assessment and remediation.

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In-Person

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295

Dual-porosity Conductive Model of Tight Sandstone Reservoir

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The tight sandstone reservoir features with multi-scale pore space and high clay content, which results in great variations in Archie's exponents. Archie's equations cannot be applied to evaluate oil and gas saturation of the tight sandstone reservoir. We proposed a dual porosity conductivity model by digital rock physics in the study. Firstly, the pores of tight sandstone are divided into macro pores and micro pores using multi-scale imaging method. The macro pores are mainly consisted of residual intergranular pores and dissolution pores, and the micro pores are mainly clay interstitial micropores and grain boundary fractures. Secondly, the 3-D gray scale images of dry samples and samples saturated by sodium iodide are obtained by X-ray computed tomography (CT). The series-parallel relationship between micro pores and macro pore are revealed by grayscale image registration and segmentation techniques. An ideal pore-throat model is established to propose the dual-porosity model for tight sandstone. Finally, the accuracy of the model is evaluated by comparing the calculation results of the model with the electrical experimental results. The results indicate the evaluation accuracy of oil and gas saturation in tight sandstone reservoirs is improved by the dual porosity model compared with the results derived from the Archie's equations.

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Energy Transition Focused Abstracts:

298

Hydraulic properties of monodisperse granular materials of different grain shape: an insight from pore-network perspective

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The hydraulic properties of granular materials are of great importance in engineering applications including earth dam protection and geothermal exploitation. These macroscopic properties are fundamentally influenced by their micro-structure. However, the understanding of the link between the microstructure and the hydraulic conductivity is still limited, especially for granular assemblies of various grain shapes. This study bridges the gap using a framework that incorporates Discrete Element Method (DEM) simulation, 3D-image processing, and pore-network analysis. Five assemblies of natural sand grains with different sphericity and roundness are generated in DEM based on imaging of real geomaterials. The 3D geometries of the assemblies are processed in OpenPNM to build their pore network, with pores taken as nodes and throats between pores taken as edges that are weighted by local hydraulic conductance. Based on complex network theory, pore network features are extracted and analysed to insight into the intrinsic links between particle shape and hydraulic properties such as hydraulic conductivity and tortuosity. The result shows the pore size, throat size, and weighted closeness centrality of the pore network are largely influenced by the particle shape.

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299

Reduced-order Modeling of Crack Nucleation and Growth in Porous Microstructures

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Understanding mechanical deformation of porous materials is important in many applications such as geologic carbon storage, geothermal energy, and energy and conversion devices such as batteries and fuel cells. Yet very little is known about how cracks nucleate and coalesce inside porous microstructures under different loading conditions. Among the various computational methods that exist in the literature, direct numerical simulation (DNS), such as finite elements, produces the highest fidelity solutions of failure. But DNS is computationally expensive, limiting their use to small samples. Discrete element methods (DEM) are popular but specialized to granular media and impose various simplifications on geometry and physics. Recently, a pore-level multiscale method (PLMM) was developed by the authors for efficiently simulating the elastic deformation of porous domains at the microscale. In this work, we extend PLMM to modeling crack nucleation and growth in complex microstructures captured by an X-ray micro-CT image. We validate PLMM against DNS under different loading conditions, including fluid-induced failure, and derive useful insights about the fracturing process itself. We demonstrate the methods capability in modeling 3D domains under triaxial loading. The results have implications for developing leak-proof protocols for injecting pressurized fluids underground and for designing durable porous materials outside of geosciences.

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MS12 / **300**

A Bounding Surface Viscoplasticity Model for Creep and Strain-Rate-Dependent Behaviour of Soils

Authors: Babak Shahbodagh[1]; Nasser Khalili[2]

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The time-dependent behaviour of geomaterials is of concern in many geotechnical engineering projects. These include the analyses of long-term settlement and creep-induced failure of infrastructure founded on soft soils, stability of natural and excavated soil slopes, strain-rate-dependent response of earth-structures subjected to dynamic loads, the construction of tunnels in squeezing grounds, and the design of geological nuclear waste disposal facilities. In this paper, a viscoplastic constitutive model is presented for the time-dependent behaviour of soils with particular reference to capturing drained and undrained creep-induced failure in clayey soils. The model is developed within the context of the bounding surface plasticity using the critical state theory and the consistency viscoplastic framework. Unlike the overstress models, the model meets the consistency condition and allows a smooth transition from rate-independent plasticity to rate-dependent viscoplasticity. The strain rate dependency of the material response is represented through defining the bounding surface as a function of the viscoplastic volumetric strain as well as the viscoplastic volumetric strain rate. A non-associated flow rule is defined to generalise the application of the model to a wide range of soils. Simulation results and comparisons with experimental data are presented to highlight the capabilities of the model.

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Energy Transition Focused Abstracts:

301

Prediction of particle deposition at the pore scale using convolutional neural networks

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Subsurface transport of colloids is of critical importance in various engineering and scientific applications, such as groundwater transport, underground H2 or CO2 storage, oil and gas reservoirs, and

geothermal energy [1]. Migration and deposition of such particles can significantly alter the physical properties of porous media [2,3]. In recent years, digital rock physics has been used to evaluate the properties of rocks at the pore scale [4]. Various numerical models can be implemented to predict flow field variations at the pore scale because of particle deposition, including continuum-based numerical models, computational fluid dynamics, Lattice Boltzmann, and pore network models. Particle tracking can be modeled by either the discrete element method or the Lagrangian approach [5]. These conventional approaches are time-consuming and require extensive computational resources. An alternative approach used here is machine learning to quickly predict the alteration of petrophysical properties of the digital rock twin. To the best of our knowledge, machine learning algorithms have not been extensively explored for predicting particle deposition at the pore scale.
This study employs convolutional neural network (CNN) architectures to predict the spatial deposition of particles in the digital twin of a granular porous medium generated using the sphere packing approach. For this purpose, we used an Eulerian-Lagrangian model of particle deposition [5] to create a dataset of porous media images at the pore scale. The spatial deposition of particles was analyzed using image-based techniques. The geometrical data augmentation was implemented to increase the size of the dataset. 80% of images were implemented for training of the network, and the rest 20% for testing purposes. The CNN model was trained on the dataset to predict precisely the spatial distribution of deposition. The input to the CNN was 2D binary images of the porous media generated by the sphere packing approach, and the CNN predictions were aimed at quantifying the spatial deposition of particles.
The results showed promising spatial prediction quality of particle deposition in the granular porous media with high accuracy. The predictions could be estimated in a fraction of a second using CNNs (a Nvidia® GeForce GTX 1080 Ti GPU with 11 GB RAM) compared to several simulation core hours by conventional CFD methods on 48 cores of an intel® Platinum 8160 CPU 21 GHz workstation (1536 core hours).

Participation:

Online

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Energy Transition Focused Abstracts:

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Lysimetric experiments to characterize the multiphase mobilization of LNAPL in contaminated soils by a multi-method monitor-

ing approach under controlled climatic scenarios.

Authors: Amélie Cavelan[1]; Fabrice GOLFIER[2]; Anne-Julie Tinet[3]; Constantin Oltean[4]; Catherine Lorgeoux[4]; Stéfan Colombano[5]; Jacques Deparis[6]; Hossein Davarzani[7]; Noele Enjelvin[8]; Pierre Faure[1]

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Light-non-aqueous phase liquids (LNAPLs) are important sources of soil contamination worldwide. Significant fluctuations of the soil bio/geochemical properties (metabolisms types, redox) and significant spatial-temporal variations of the pollutant saturation distribution occur on the LNAPL different phases (pure phase, dissolved, residual, entrapped droplets). These fluctuations are often strengthened by the multiple imbibition/drainage cycles caused by groundwater level variations that affect the three-phase fluids distribution in the soil (LNAPL, gas, and water) and the LNAPL release rates towards the dissolved and the gaseous phase [1,2]. Hence, the real LNAPL soil saturation distribution cannot be easily inferred from the thickness of LNAPL in monitoring wells, complicating the contamination characterization and the remediation actions, often long and costly. For these reasons, monitoring methods need to be improved to better characterize the contamination in integrating both the multi-compound and the multi-phase aspects. The relation between the LNAPL mobilization mechanisms and the groundwater level dynamic need also to be further understood, especially in the climate change context where increased groundwater fluctuations are expected [3]. For this purpose, we instrumented two lysimetric soil columns (2 m3) contaminated with LNAPL. The device combines in-situ monitoring (electrical permittivity and conductivity, soil moisture, temperature, pH, RedOx) and direct sampling and measurements in monitoring wells, gas collection chambers, and suction probes. This equipment allows the assessment of the multi-component and multi-phase LNAPL release (pure, dissolved, and gaseous phases) and soil saturation distributions (electrical permittivity and conductivity) under controlled scenarios of precipitation and groundwater fluctuation patterns. The dissolved, gaseous, and pure LNAPL phases were characterized in the lab by GC-MS and field µGC technics. Meanwhile, 1D column experiments allowed the determination of the soil hydrological properties during LNAPL/water/air imbibition/drainage cycles. Our first scenarios (120 days of monitoring), shows that the coupling of physical-chemical, geophysical, and hydrological monitoring methods allows a global characterization of the contamination and its behavior during groundwater table variation scenarios. This experiment also demonstrated that increasing the groundwater level variation intensity accentuates the spreading and trapping of the pure LNAPL phase across the soil porosity, which favors LNAPL volatilization and dissolution processes. These findings will allow to better identify and combine key LNAPL processes to improve models and strengthen the recommendations concerning the characterization and monitoring programs for hydrocarbons polluted sites.

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Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-A / 303

NAPL dissolution and transport in porous media: Upscaling the Mass Exchange Coefficient

Authors: Narges Dashtbesh[1]; Anne-Julie Tinet[2]; Fabrice GOLFIER[3]; Constantin Oltean[1]; Michel Quintard[4]

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Understanding and modelling contaminant transport is necessary to assess pollution sources'lifetime and severity and optimize the remediation strategies. The transfer of contaminants from the NAPL (Non-Aqueous Phase Liquids) phase to the aquifer is a multi-scale problem with different transport mechanisms within the various phases and at the interfaces. This two-phase flow problem is, in particular, driven by mass transfer between both phases, and is generally described by local non-equilibrium models. Such models at the macroscopic scale include transport equations for each phase which are coupled through one or several mass exchange coefficients. While these coefficients, which integrate the impacts of different pore-scale features (pore geometry, phase distribution, flow velocity), play a key role in the fate of the pollution source, it is usually approximated, for a given phase saturation, by a constant value estimated from empirical correlations (Quintard and Whitaker 1994, Soulaine et al., 2011). However, it generally shows a transient behaviour and can evolve with NAPL phase composition and relative solubilities, which remains poorly studied (Shafieiyoun & Thomson, 2018).
In this work, we start with the numerical modelling of the problem at the pore scale using COMSOL Multiphysics. The NAPL phase is considered an immobile blob at the pore centre and is composed of a non-soluble component and one or more soluble components. At this scale, the dissolution is implemented using Raoult's law at the interface between phases. The solubilities evolve in a complex and coupled way as a function of the mass fractions of the considered components, themselves dependent on time. The change in the NAPL's volume is modelled using an ALE approach and the derived equation for the interface velocity. Flow and transport in the water phase are considered and transport in the NAPL may be taken into account. We study the impact of different factors (number of soluble components, component diffusions, interface evolution, Péclet number) on the form and behaviour of the mass exchange coefficient. In the second step, we upscale from the pore scale to the Darcy scale using a numerical approach, with a focus on the mass exchange coefficient. The potential implications of replacing this time-and-space-dependent mass transfer coefficient in a Darcy-scale model with a constant and unique value as well as with a function of different state variables are discussed.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 306

Digital concrete physics: Prediction of the effective elastic material properties of concrete by pressure-dependent high-resolution X-ray Computed Tomography

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Over the past three decades, digital rock physics (DRP) has become a complementary part of the field of study to understand better the behavior of porous media at the micro-scale. In this study, we apply the established five-step DRP workflow to a concrete specimen (e.g., Wildenschild et al. 2002; Schlüter et al. 2014) : (1) Preparation of a high-resolution X-ray computed tomography (XRCT) volume, (2) tomographic reconstruction, (3) assessment and handling of the X-Ray artifacts (4) segmentation of pore and grain phases, respectively, and (5) solving equations due to the demanded properties.

Previous studies have shown that under elevated pressure conditions, XRCT can only provide visual evidence of compression under favorable conditions due to sub-resolution changes, while ultrasonic velocity measurements, for example, indicate compression of the porous medium more clearly (e.g., Madonna et al. 2012; Saenger et al. 2016; Liang et al. 2021). Therefore, we apply the results to a concrete specimen based on the published experience with pressure-dependent XRCT of rocks.

Our XRCT scans were performed under confining pressure conditions with a purpose-built X-ray-transparent pressure cell (Lebedev et al. 2017) at 0.1, 6.5, 13, 26, 36, and 46 MPa. After image post-processing, i.e., filtering and gray-scale threshold segmentation based on thin sections, the pore,

and solid phases are analyzed qualitatively and quantitatively to predict the extent of potential compaction at elevated pressure conditions. Finally, the effective elastic material properties are modeled based on the segmented volumes at different pressure conditions and compared with the corresponding laboratory measurements for larger samples.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS08 / **307**

Pore-scale investigations of two-phase flow on mineral reaction rate

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In various subsurface systems, the interactions between multi-phase flow and mineral reactions play an important role in controlling the evolution of porous media. These interactions - especially the impacts of multiphase flow dynamics on mineral reaction rates - are rarely accounted for in continuum scale models, or are simply corrected via reactive surface area and saturation of the aqueous phase. However, the relations (e.g., power laws between reactive surface area and water saturation),

used for the correction are not based on pore-scale dynamics. Our previous study of a single channel with different levels of roughness showed that the mineral reaction rate in a gas bubble flow is significantly reduced compared to a single-phase flow system at the same flow rate. The extent of reduction in reaction rate follows a non-monotonic relationship with respect to water saturation, in contrast to the traditionally-used monotonic relationship (i.e., a power law relationship). In this study, we extend our investigations to pore-doublet geometries, to examine how two-phase flow dynamics arising from competing channels as would be expected in complex porous media affect mineral reaction rates. For our investigations, we control the two-phase flow dynamics by varying the air and water flow rates (i.e., capillary number) and the relative difference between the competing channels. Calcite dissolution rate in these channels is quantified for the two-phase flow cases with different saturations and the corresponding single-phase flow case. The relationships between the changes in dissolution rate in two-phase flow cases and the wetted surface area, the interfacial area, and water saturation are examined to provide insights on improving reaction rate descriptions in multiphase continuum scale models.

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Energy Transition Focused Abstracts:

308

Effect of Dihydrogen Phosphate Anion in Smart Waterflooding through Zeta Potential Measurements and Coreflooding Simulations

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Smart waterflooding is an enhanced oil recovery technique that has gained great attention in the latter decades. It consists of tuning the ionic composition of the injected water, to improve the microscopic displacement efficiency. Hence, the effectiveness of this method strongly relies on the understanding of chemical interactions between the crude oil, brine and the rock. In this study, we analyze the brine-rock interactions via simulation of coreflooding experiments using surface complexation modeling. We investigate the impact of dihydrogen phosphate ($H_2PO_4^-$) anion in the calcite-brine interface alteration.

We develop a surface complexation model in geochemical open-source software, PHREEQC to history match experimental zeta potential measurements, by tuning thermodynamic parameters of adsorption equilibrium. Laboratory measurements of zeta potential were conducted with pure calcite;

tested brines were seawater (57614.3 ppm) with varying dihydrogen phosphate concentrations (0-1000 ppm). Zeta potential measurements were conducted via phase-analysis light scattering. Then, we couple the surface complexation model with a 1D advection-reaction-dispersion model to simulate coreflooding experiments using PHREEQC. We used the core petrophysical properties from a carbonate reservoir to account for dispersion. In our geochemical model, we consider dissolution of calcium carbonate, bulk aqueous speciation, dispersion and surface complexation on calcium carbonate surface.

Adding dihydrogen phosphate to seawater shows a positive impact on wettability alteration, observed by the change of contact angle between oil and carbonate as well as drop in zeta potential. The surface complexation model matches experimental zeta potential measurements with a good accuracy. Carbonate rocks are highly heterogeneous; therefore, they have high hydrodynamic dispersion. This is observed in the sigmoid-shape curve for chloride, which is treated as tracer in our simulations. This is in agreement with coreflooding behavior for carbonates. Coreflooding simulations show calcium carbonate dissolution. In addition, injection of dihydrogen phosphate exhibits precipitation of hydroxyapatite. During coreflooding simulations, the injected brine decreases zeta potential in the core. These findings may indicate wettability alteration in the core. We will further compare these coreflood simulation results to experimental coreflooding tests.

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Energy Transition Focused Abstracts:

Poster / 309

Bacteria and surfactants for bio-cemented foams

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Co-authors: Vincent Langlois [1]; Marielle Guéguen-Minerbe [2]; Daniel Grande [3]; Sébastien Vincent-Bonnieu [4]; Olivier PITOIS [1]

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Microbially-induced carbonate precipitation (MICP) may be used to improve soil strength. The method relies on the total or partial saturation of the porous medium with a calcifying bacterial suspension. The project presented here focuses on filling the porosity of granular packings using bacterial liquid foam in order to achieve low liquid saturation. In addition to saving liquid, the foam would allow the bacteria to be strategically located, *i.e.* at contacts between grains, which is expected to improve the process.

However, this approach raises the issue of the compatibility of the bacteria with the surfactants used to stabilize the foam. The challenge is to maintain the ability of bacteria to induce carbonate (CaCO3) precipitation in their environment while evolving in a high content of surfactants. Most surfactants are used as cleaners. Although they commonly have antimicrobial properties, some of them are well tolerated by bacteria.

In this study, we focused on two families of surfactants: saponin and alkyl polyglucosides, i.e. CXM or CXG, with X = number of carbons, M = maltoside, and G = glucopyranoside. These surfactants were tested with two bacterial strains, namely *Sporosarcina pasteurii* (*SP*) and a strain similar to *Bacillus haynesii* (*BH*).

The choice of formulation was based on the study of several parameters: bacterial activity and growth, pH variation, and CaCO3 precipitation.
When monitoring the bacterial activity and growth of the two strains, samples with C8G or C10G showed much lower activities than those for the control sample (without surfactants). These surfactants inhibited bacterial growth and activity. On the other hand, for samples with C8M, C10M or saponin, bacterial activity and growth were substantially above those associate with the control sample. They increased the bacterial activity because the bacteria degraded these molecules, as revealed by high performance liquid chromatography. Therefore, it appeared that the response of bacteria to APG surfactants was highly dependent on the molecular structure of the APG: bacterial activity was optimal when the carbon chain was the shortest and the hydrophilic head was the largest. However, the experiments with C8M and the *BH* strain showed variations in pH towards an acidification of the medium, which was not suitable for the precipitation of CaCO3. The study of bio-carbonation in the presence of C8M (only with *SP*), C10M, and saponin surfactants showed a sufficient rate of calcification to consider consolidation of a granular packings. Combining all the results, the most convenient surfactants for the precipitation of CaCO3 were found to be C10M, C8M, and saponin.

Besides, the study of the liquid permeability of the foams confined into the porosity of the granular packings showed that APGs allowed for an easier delivery of the nutriments though the medium, as compared to saponin. Therefore, we provided all the information needed to approach granular column calcification tests.

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Energy Transition Focused Abstracts:

MS05 / 310

Microfluidic and numerical investigation of anisotropic permeability alteration during biomineralization in porous media

Authors: Felix Weinhardt[1]; David Krach[2]; Jingxuan Deng[3]; Johannes Hommel[2]; Holger Class[2]; Holger Steeb[4]

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Biomineralization, e.g. enzymatically (or microbially) induced calcium carbonate precipitation (EICP) is a promising geo-engineering method with the potential, for example, to seal leakage pathways in the subsurface or to stabilize soils. It is associated with an alteration of porosity and, consequently, permeability. A major source of uncertainty in modelling EICP is in the quantitative description of permeability alteration due to precipitation, based on commonly applied porosity-permeability relations [1]. To improve these relations for REV-scale models, we investigate the effect of EICP on hydraulic properties in microfluidic experiments by measuring the pressure drop to calculate the permeability and by observing the pore-space alterations with optical microscopy. The experimental setup and procedure are described in [2]. The results of the presented study show that preferential flow paths can form under continuous flow conditions and ongoing precipitation [3]. Our aim is to analyze this effect of strong local inhomogeneity for REV-scale permeability. We expect to quantify this as anisotropy also in pore-scale numerical investigations based on the images obtained from optical microscopy.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS08 / 311

Advective trapping in the flow through composite heterogeneous porous media

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We study the mechanisms of advective trapping in composite porous media that consist of circular inclusions of distributed permeability embedded in a high conductivity matrix. Advective trapping occurs when solutes enter a low velocity zone in the porous medium. Current multirate mass transfer (MRMT) models consider slow advection and diffusion but do not separate these processes, which makes parameterization difficult. Transport is analyzed in terms of breakthrough curves measured at the outlet of the system. We observe that the volume fraction occupied by the inclusion controls the curve's peak behavior, while the distribution of permeability is responsible for the shape of the tail. Using the continuous-time random walk framework, we derive a Lagrangian trapping model parameterized in terms of volume fraction and the distribution of conductivites in the inclusions. Then we show that this model is equivalent to a first-order MRMT and to a non-local partial differential equation for the mobile solute concentration derived by volume averaging of the microscale transport equation. The upscaled approach, parameterized by medium and flow properties captures all features of the observed solute breakthrough curves, and sheds new light on the modeling of advective trapping in heterogeneous media.

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Energy Transition Focused Abstracts:

Poster / 312

Impact of structural heterogeneity on fluid phase patterns in two-phase flow through two-dimensional porous micromodels

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The fluid phase saturation degree is often used to define multiphase flow conditions in porous media macroscopically. However, the microscopic (pore-scale) fluid phases'distribution pattern can be crucial and is usually not measured or quantified. For example, the topology and connectivity of the fluid phases impact the permeability and, thus, relative flow rates. Therefore, they will impact multiphase flow and related transport processes, including water leaching and drying in soils and the vadose zone, enhanced oil recovery, and CO_2 sequestration in deep geological formations. These processes will, in turn, impact the fate of nutrients and pollutants in the subsurface, the precipitation and dissolution of minerals, and the extent of microbial activity, to name a few. Still, the link between the porous medium's structure –the distribution of pore sizes and their relative positions – and the pore-scale fluid phase distribution during multiphase flow is still far from being understood. An essential requirement, at least experimentally, is to obtain direct observations of the displacement patterns. To this end, we use micromodel experiments with quasi-two-dimensional porous

media. The samples are created from numerically generated geometries of circular posts positioned in a Hele Shaw-type flow cell and fabricated in PDMS. We vary the medium's heterogeneity by controlling the disorder in the circular posts'diameters and the correlation length of their spatial distribution. In the experiments, we simultaneously inject liquid and air to establish an unsaturated flow pattern with a connected liquid phase cluster. The liquid phase contains a fluorescent dye, and the flow cell is illuminated to excite the dye at the appropriate wavelength. We take images of the emitted light intensity and analyze them to determine the fluid phase clusters'location and geometric characteristics. We infer their number, position, area, and liquid-air interface length. In addition, we calculate the clusters'Minkowski functionals. We find that increasing the spatial correlation length of the posts (or, equivalently, pore sizes) decreases the number of air (the non-wetting phase) clusters while increasing their average area, perimeter length, and distance to the closest neighbor air cluster. In addition, the roughness of the air-liquid interface is smaller for longer correlation lengths. These characteristics impact the connectivity and tortuosity of the connected liquid (wetting) phase and could influence the liquid flow characteristics and, thus, solute transport and mixing processes. Our experimental study could also be used as a basis for a deep learning approach to derive more generalized relationships between porous medium structure and fluid phase distribution.

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Energy Transition Focused Abstracts:

MS13 / 313

Multiphysical pore-scale modelling of ion transport in variably saturated nanoporous media

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The transport of solutes in partially and fully saturated nanoporous media such as compacted clays and tight rocks is a very fundamental process related to contaminant transport in groundwater and radionuclide migration in the context of nuclear waste disposal. Specifically, the charged surfaces of minerals induce an electrical double layer (EDL) in the electrolyte by the long-range Coulomb force and therefore influence the ion distribution within nanopores. The EDL overlap within nanopores can magnify the impact of the two-way coupling between electrokinetic effects and ion diffusion. A novel pore-scale numerical framework was developed to simulate ion transport in partially and fully saturated nanoporous media with consideration of the EDL and thermal effects. This numerical framework directly solves coupled Poisson-Nernst-Planck equations by the Lattice Boltzmann method (LBM) on GPUs, which can automatically capture the structure of the EDL in nanopores. In fully saturated conditions, the present study quantitatively characterises the influence of the EDL

on ion diffusion in compacted clays under different situations. It is indicated that the normalized volume charge density has a significant impact on ionic tracer diffusion. In clays with a large normalized volume charge density, the EDL has a major impact on ion diffusion. When the ionic strength of the pore solution and temperature are constant, the flux from the electromigration term can be negligible. However, once a gradient in ionic strength or temperature is added, the electromigration process should be considered carefully due to its non-negligible role to balance the alteration of total flux. For the ion transport in partially saturated nanoporous media, the liquid-vapor distribution is given by the Shen-Chen LBM in the pore network. Our pore-scale simulations show that the thin water films on the surface of clay particles have non-negligible influences on ion transport under the condition of low saturation. The present study could help to improve the understanding of the mechanisms of ion transport in partially and fully saturated nanoporous media.

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Energy Transition Focused Abstracts:

314

An efficient and robust fully implicit pore-network model for the pore-scale simulation

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Pore-network model (PNM) aims to capture pore-scale phenomena in a computational efficient manner with the help of simplified porous media geometry. Quasi-static PNM focuses on capillary driven flow in the system near the equilibrium state, while dynamic PNM takes also the impact of viscous forces into account to compute transient flow.
System of free-flow coupled with porous medium flow is ubiquitous in natural applications (e.g. the evaporation of water from partially saturated soil as wind flowing over). To simulate the flow in the porous medium in such coupled systems, fully implicit dynamic PNM is suitable. That is because it doesn't impose restriction on the time step size during solving the flow, which is normally required by different explicit and semi-fully implicit pore-network algorithms[1][2].
In this study, we introduce a fully implicit pore-network model and discuss the related modeling and numerical challenges. One main challenge is to deal with the discontinuity occurring in local relative permeability of phases due to invasion and snap-off in the pore-throat. This discontinuity causes convergence issues during the simulation. To handle this, we propose approaches such as different kinds of regularization strategies. Furthermore, the new scheme is verified and validated for different test cases.

Participation:

Online

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Energy Transition Focused Abstracts:

Poster / 315

Effects of microplastics on temperature profiles inside porous media during evaporation

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The increase in plastic production is expected to exacerbate plastic waste disposal in terrestrial ecosystems. Soil represents a large reservoir for plastic wastes. Once disposed into the soil, plastic wastes interact with soil particles and biota and affect chemical, physical, and biological processes in soil (Jannesarahmadi et al., 2023). Microplastics (MPs) with distinct thermal and radiative properties and filling characteristics can alter energy partitioning over the surface of drying porous media and thus subsurface thermal regimes. The present study aims to quantify impacts of MPs on latent heat loss and temperature dynamics in drying sandy media. We conducted a series of evaporation experiments on sand columns (height: 20 cm –diameter: 8 cm) with grain size ranging from 0.4 to 0.8 mm and density of 2.65 g/cm³. Two types of microplastics with different characteristics and concentrations were used: Polyethylene (PE) with 34 to 50 μm particles and density of 0.94 g/cm³ and Polyvinylchloride (PVC) with particles ranging from 80 to 200 μm and density of 1.4 g/cm³. Mass loss rates from sand samples with different concentrations of MPs (i.e., 0.5, 2, and 5%) were compared with drying rates of the sand column without MPs serving as a reference. An array of thermocouples continuously measured vertical temperature profile in drying sand columns subjected to different wind and radiative boundary conditions. Airflow was generated by an adjustable fan and shortwave radiation flux was mimicked using halogen lamps with different intensities. Our preliminary results show that the presence of MPs with different characteristics alter evaporative loss and vertical temperature profiles in drying sand samples with the surface accumulation of PE particles (with lower density relative to water) influencing the thermal and radiative properties at the surface of drying porous media. The study provides new insights into the impact of MPs on energy partitioning dynamics over drying terrestrial surfaces and subsurface thermal regimes that could potentially affect various hydrological and biological processes in soil.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS11 / 316

A lab on a chip concept for rationalizing hydro-geochemical processes at the pore scale

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Hydro-geochemical processes such as transport-induced mineralization are important processes governing the evolution of many systems in the context of energy-related exploitation of the sub-surface. These processes can lead to an alteration of permeability, diffusivity and other physical characteristics of the rock matrix that can have significant effects on subsurface solute and gas transport. The understanding of these phenomena at the pore scale is a prerequisite for the development of predictive conceptual approaches to describe the evolution of the subsurface. Our lab on a chip concept which combines microfluidic experiments and reactive transport modelling [1, 2] has proven to be a powerful tool to (i) evaluate the impact of hydrological heterogeneity on nucleation mechanisms [3], (ii) decode oscillatory zoning exhibited by solid solutions crystallizing in porous media [4], (iii) unravel the dynamic nature of porosity clogging at perturbed interfaces [5], and (iv) parameterize porosity-diffusivity relationships [6] with respect to coupled mineral dissolution-precipitation reactions. At present, we resolve current controversies on crystallization in confinement addressing specifically whether nucleation is pore size dependent.
Our investigation focuses on one of the most problematic minerals, barite, encountered in energy-related sub-surface exploitation [7]. Microfluidics experiments conducted in nano-confined volumes of solution, i.e., in droplets ranging between 0.3 and 3 nL, showed that nucleation is a probabilistic event that scales with the volume of fluid. While our statistical analysis shows that inhibition of barite nucleation will start at pore sizes < 1 μm, theoretical calculations show that the pore size-controlled solubility [8] effect (a thermodynamic effect) becomes effective only in pores of sizes less than < 0.1 μm. In a second step, the influence of diffusive transport was also investigated by fostering the crystallization of barite in a pore network consisting of large and small micrometer-sized pores interconnected by fine squared capillaries of 1 um2 cross-sectional area. Although preferential mineralization was observed in larger pores, at low supersaturation crystallization was observed only in the fine capillaries. This unexpected behaviour can be explained by the high reactive surface area (and defects) per unit volume resulting from in an increase in nucleation sites in the capillaries. The general conclusions of our study are that in porous media the nucleation kinetics of barite is more and more affected by the surface energy of the substrate as the pore size decreases from micrometric

to nanometric scale. Consequently, it can be expected that mineralization occurs preferentially in larger pores in rock matrices but other parameters such as (i) exchange of the fluids w.r.t reaction time, and (ii) the shape, roughness, and surface functional properties of the pore should also be considered as they might reverse this trend.

Participation:

In-Person

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Poster / 317

NMR Study of water transfer from bio-based materials to the living plant

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In the context of climate change, studies of water transfer in bio-sourced materials are becoming essential in order to meet the multiple challenges of developing high-performance materials over the long term and preserving resources while limiting greenhouse gas emissions. One of the keys to supporting these studies is access to the "water status" in these porous materials [1]. However, the monitoring of their performance over time is often limited to destructive studies or relies on techniques that are too local or average, or even intrusive.

Here, we present the development of an innovative methodology based on nuclear magnetic resonance (NMR) relaxometry and imaging (MRI) at low and high magnetic fields, respectively, to study water content and transport during water stress in living materials, from the leaf to the whole plant scale. The results obtained by the combination of these approaches will be compared with water transfers in model porous materials such as wood, cellulose, glass beads, etc. Indeed, thanks to NMR approach, it has been possible to identify the drying mechanisms in wood and to show that bound water plays a fundamental role, transporting, by diffusion, free water from the interior of the material to the free surface, and this during all the drying phase [2]. Another interesting result concerns the behavior of NMR signal and relaxation times in two contrasted genotypes in term of cellulosic ratio. This dependence of relaxometry provided an important information on molecular dynamics directly related to plant resistance [3].

This study has demonstrated the potential and the versatility of NMR relaxation as a means to characterize the microstructure of living porous material and model water transport mechanisms under different environmental constraints.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 319

Quantifying shrinkage of natural clay samples with an automated high-frequency measurement set-up

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Shrinking and swelling of expansive clay deposits can cause severe damage to infrastructure (Mokhtari & Dehghani, 2012). Volume change depends on the characteristics of the porous material, such as clay content, mineralogy, organic matter content, soil moisture conditions and drying history (Basma et al., 1996 ; Boivin et al., 2004; Puppala et al., 2007). However, predicting the shrinking and swelling of natural clay deposits as a function of material properties and soil moisture conditions is not yet possible. Measuring shrinkage and swelling of natural, undisturbed clay samples in a controlled laboratory setting will provide information on the shrinkage behaviour in the field and can be used to establish models.

To quantify shrinkage and swelling of shallow clay deposits, we have designed a new measurement set-up based on the HYPROP 2 measurement device (UMS, 2012; Schindler et al., 2015), using cylindrical samples (height: 5 cm, diameter 8 cm). The set-up is designed to create minimal disturbance to the samples during air drying in a climate-controlled room, while measuring volume, water content and soil water suction every 10 minutes. The volume measurements are carried out with 5 optical distance sensors that measure the distance to the samples from a rotating robot arm. Distance to the samples is measured at 15 points per sample on the top and 10 from the side while moving along the sample. The distance between measurement points varies between 0.5 (on top) and 0.8 cm (from the side). These point data are converted to volume measurements, assuming cone shaped samples.

The first experiment aims to distinguish shrinkage behaviour of differently prepared samples and to confirm the likeness between three similarly prepared subsamples. In total 8 samples were extracted at 1.5 m depth from a fluvial clay deposit. These samples were saturated for half a year with different solutions: tap water, an instant ocean mix (Cl 16.9 g/L; Ca 0.388 g/L) and a saline calcium solution (Cl 6.20 g/L; Ca 4.76 g/L). The measurements yield a detailed overview of the shrinkage behaviour. Total shrinkage differs within the triplicates up to 1.3% (tap water), 3% (instant ocean solution) and 4.6% (saline Ca solution). The samples saturated with tap water and instant ocean mix totally shrink 42-44%. The samples prepared with the saline Ca solution show similar shrinkage rates to the instant ocean mix samples for the first two weeks of drying. Thereafter, the shrinkage rate of the saline Ca samples declines, resulting into a cumulative shrinkage of 36%.

The experimental set-up is able to capture the different shrinkage rates of the differently prepared samples. The shrinkage rates of the duplicate and triplicate samples agree well, with a maximum shrinkage difference of 4.6% between triplicates. These are very small differences considering that all samples are natural clay sediments without any form of homogenization. Currently, we are investigating the reversibility of the shrinkage and swelling. These results will be used to test a shrinkage-swelling model.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS04 / 320

Magnetic resonance imaging of the swelling of polymeric hydrogels

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Superabsorbent polymer hydrogels are a class of porous media with only two phases (solid and liquid) that have the ability to swell more than 200 times their original volume when placed in water. This feature stems from its unique structure which consists of long polymer chains linked together in a weakly cross-linked network, and the presence of hydrophilic sites along the polymer chains. During swelling, water molecules come to occupy the hydrophilic sites, resulting in an expansion of the polymer network. The cross-linking of the polymer chains, although weak, prevents the structure from breaking at high water contents and gives the hydrogel a certain rigidity. Due to the ionic nature of hydrogels, their swelling is generally accompanied by complex mechanisms involving electro-hydro-chemo-mechanical couplings [1]. When a spherical bead of dry superabsorbent polymer is immersed in water, a transient phenomenon of gel formation is observed on the surface of the bead with the appearance of lobes, then their coalescence, finally resulting to the same spherical geometry than the original bead but filled with water [2].
The MRI technique, sensitive to the presence of water molecules, is an interesting means to study the swelling of hydrogels and the associated coupling phenomena. However observing by MRI the behaviour of a hydrogel immersed in a volume of water is not an easy task because the fully swollen hydrogel contains more than 99% water. It is therefore difficult to distinguish its interface from the water in which it bathes. It is thus necessary to add a contrast agent (paramagnetic Cu2+ ions for instance) to differentiate the NMR relaxation parameters of the solution and the hydrogel [3]. But the presence of ions in solution can also significantly affect the hydrogel swelling phenomenon.
A preliminary study was carried out to evaluate the swelling of hydrogel beads (polyacrylamide) immersed in copper sulphate solutions at different concentrations. This type of hydrogel has a strong tendency to capture Cu2+ cations. This adsorption leads to additional cross-links between the polymer chains, which can greatly reduce the swelling capacity of the hydrogel. NMR images were then taken to describe the swelling kinetics of these hydrogel beads immersed in aqueous solutions of CuSO4. For this, we used an NMR spectrometer (Bruker 600 MHz Wide Bore) equipped with a micro-imaging device. These experiments allowed us to follow the swelling of the hydrogel beads over time: the formation of the gel on the surface of the polymer bead, the gradual disappearance of the solid polymer core, the appearance then the coalescence of the lobes, and the return to a spherical geometry of the water-swollen hydrogel. For the tests carried out at high concentrations (Cu2+ >1 mM), complex mechanisms are observed coupling the diffusion and adsorption of Cu2+ ions in

the hydrogel. It is even possible to observe, after a first swelling phase, a second phase of shrinking associated with an osmotic drying of the hydrogel.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS21 / 321

The role of temporal and spatial fluctuations for scalar transport at the interface between a free turbulent flow and a porous medium

Authors: Simon v. Wenczowski[1]; Michael Manhart[1]

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Exchange processes at the interface between a porous medium and a turbulent flow field are relevant in a wide range of natural and industrial systems: Prominent examples for technical applications range from food drying up to processes within fuel cells. In the environment, the exchange of mass within the hyporheic zone is vital for the health of aquatic ecosystems, whereas the evaporation from soils must be considered for sustainable land use. Despite the apparent heterogeneity of these fields, scalar transport across the interface is driven by a common set of mechanisms, which can be distinguished in the double-averaging framework (e.g. [1,2,3]): Whereas transport due to molecular diffusion requires gradients in the scalar concentration field, turbulent scalar transport results from correlated fluctuations of the flow and scalar field *in time*. In contrast, dispersive scalar transport is caused by correlated fluctuations of the mean flow and scalar field *in space*.

The objective of our research is to contribute to a more comprehensive mechanistic understanding of scalar transport in the interface region. We (i) identify the regions of influence of individual scalar transport processes and (ii) analyze the interaction between the fundamentally different processes within the double-averaging framework.

For the numerical investigation with our in-house code MGLET [4,5], the porous medium is represented by a static random pack of spheres with uniform diameter. While the advection-diffusion equation is solved for a passive scalar with a Schmidt number of $Sc = 1$, the flow field is obtained from solving the incompressible Navier-Stokes equations. By means of a single-domain Direct Numerical Simulation (DNS), all temporal and spatial scales are resolved both in the free flow region and in the pore space of the porous medium, which avoids any model assumptions. For a representative case, the flow field is validated against experimental data [6]. In total, we consider eight different

simulation cases with shear Reynolds numbers in the range of $Re_\tau = 150$–500 and permeability Reynolds numbers of $Re_K = 0.4$–2.5.

Instantaneous fields (please, find figure attached) provide an intuitive impression of the processes, which is supported and quantified by the double-averaged statistics of the results: Whereas turbulent scalar transport dominates in the free flow region, dispersive scalar transport takes the leading role in the topmost sediment layers below the interface, before molecular diffusion becomes most relevant in deeper regions. The results confirm that the relative importance of different processes is determined by Re_K [7]. Observing that turbulent and dispersive scalar transport hardly co-exist in any regions, we evaluate budget equations for temporal and spatial fluctuations in the scalar concentration field to explain the interaction between the two processes.

The obtained insight is meaningful for the development of hyporheic scalar transport models, as the described interaction prohibits addressing the problem as a mere superposition of two transport processes. Also, ecological implications can be derived, as the presence or absence of strong spatial mean concentration gradients influences the biocenosis in a habitat.

Participation:

In-Person

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Poster / **322**

Bacterial chemotaxis in heterogeneous porous media in the presence of nutrient hot spots and flow

Authors: Maximilian F. Stoll[1]; Roman Stocker[2]; Joaquin Jimenez-Martinez[3]

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Subsurface porous systems, like soils and aquifers, are physically and chemically highly heterogeneous. Especially on the microscale, chemical hot spots and heterogeneous pore-sizes, which lead to a wide range of fluid flow velocities and strong local gradients, control the physico-chemical landscape. Microorganisms capable of biasing their motion to swim along these chemical gradients – known as chemotaxis –profit from their ability to navigate towards nutrient hot spots, such as contaminant droplets, soil aggregates or plant roots. This ability and their ubiquitous presence in natural subsurface systems gives them an important role for triggering reactions on the pore-scale for the availability of nutrients, the degradation of contaminants or soil respiration.
We developed a novel experimental microfluidic platform to study chemotaxis in the presence of chemical hot spots in porous media under flow conditions. In this multi-layered polydimethylsiloxane (PDMS) device, hydrogel features are embedded into the porous medium, acting as diffusive point sources. The experimental platform is giving both, full optical access to the pore-space and spatio-temporal control over the physico-chemical landscape. The nutrient plumes formed downstream of the hot spots under flow drive the swimming of chemotactic bacteria. By tracking the swimming of single cells under different flow conditions, we can link the bacterial behaviour to physical, chemical and hydrodynamic heterogeneities. This enables the study of the response of chemotactic bacteria to pore-scale chemical gradients and sheds new light onto the transport of microorganisms in the subsurface.

Participation:

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MS08 / **323**

Sorption in heterogenous porous media: a numerical study of the effects of spatial heterogeneity of pore structure

Authors: Mohaddeseh Mousavi Nezhad[1]; Milad Hosseini[None]

[1] *Associate Professor*

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We present a computational model to simulate both adsorption and desorption processes interactions with hydrodynamics. Flow and mass transport equations and various sorption kinetic equations are solved with Lattice Boltzmann method. The computational developments are used for direct numerical simulation of flow and transport in three-dimensional digitized soil samples and are supported

and validated by experimentally measured data. The model allows to include the details of contact surface between adsorbate and adsorbent for computation of sorption rates within porous media. This modelling approach not only enables an important mechanism to be simulated for real-life applications, but also provides an enabling computational framework within which the fundamentals of sorption can be studied. The simulation data are used to drive mathematical formulations that predict macro-scale sorption rates based on tortuosity of fluid paths, pore velocity distribution and Peclet number.

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MS06-B / 325

The Influence of Viscosity and Wettability on Immiscible Fluid Displacements in Porous Media

Authors: Harris Rabbani[1]; Saideep Pavuluri[1]; Ran Holtzman[2]

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We study the synergistic impact of wettability and viscosity on immiscible fluid displacements in heterogeneous porous media. Direct Numerical Simulations are performed for viscosity ratio M (of invading vs defending fluid) ranging several orders of magnitude and contact angles ranging from very small to very large i.e. from completely wetting to completely non-wetting. The capillary number is kept constant at ⊠⊠=1×10−6 for all the investigations.
We notice different fluid displacement patterns such as fingering and compact displacements when the Ca is maintained low and by varying the viscosity ratios and the contact angles. For viscosity ratios greater than 1, the morphology of the displacement patterns is observed to be compact and is hardly affected by the wettability. On the other hand, at viscosity ratios lower than 0.1, we observe viscous fingering during imbibition and drainage. When the viscosity ratio moves towards 1, capillary fingering emerges. This intriguing observation suggests that one cannot use the knowledge about the displacement patterns to comment on the wettability states of the porous medium.
We further quantify the pore occupancy by the invading fluid during imbibition and drainage. Though we notice similar displacement patterns that occur at lower (M<1) and higher viscosity ratios (M>1), we notice differences in the pore filling mechanisms by the invading fluid. For M>1, the 'co-operative pore filling'is prominent irrespective of the wettability state. For M<1, we notice the dominant pore invasion mechanism during drainage is 'channelling'whereas for imbibition, the wetting phase propagates over the surface of the solid grains gradually.

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Energy Transition Focused Abstracts:

MS20 / **327**

Data-integrated tracer transport simulations in brain tissue: vascular networks, perivascular spaces, extra-vascular tissue

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Tracer experiments are used to assess the transport of solutes and water in brain tissue. Only sparse information is available about the mechanisms and major pathways of water and some solutes entering (infiltration, perfusion) and leaving (clearance) the functional brain tissue. Moreover, there are three main issues with current experimental data when it comes to the quantification of transport: (1) the
underlying anatomy and transport pathways are complex (e.g. microvascular networks)
but is believed to be crucial in facilitating transport, (2) the measured
tracer transport is usually only a proxy of what we are interested in (e.g. water transport), (3) the tracer transport can often not be assessed directly but is to be inferred from a proxy signal (e.g. NMR signal or fluorescence microscope image).

In an attempt to bridge scales, fill in missing data, and connect various data sources, we present a mathematical model to perform virtual tracer perfusion simulations in brain tissue. We consider the architecture of microvascular networks [1] and a parametrization of the model based on a combination of experimental data and computational estimation [2]. The mathematical model is a three-compartment model (vascular, para-vascular, extra-vascular) formulated as a coupled mixed-dimensional system of partial differential equations. Advanced discretization techniques [3] and software [4] for flow and transport in porous media with embedded transport network systems allow for simulating domains with thousands of blood vessels.

In comparison with two-photon microscopy image data in live sleeping and awake mice [5], we discuss the role of compartmentalized molecular diffusion and dispersion driven by arterial pulsations. We show that due to the low volume fraction of the perivascular space, transport into the tissue only appears enhanced if there is a significant mixing effect due to arterial pulsations. We discuss major difficulties arising when comparing simulation results to the image data and demonstrate how image data may be subject to misinterpretation in a lack of careful consideration of supporting information in the imaging process.

Participation:

In-Person

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Energy Transition Focused Abstracts:

328

An experimental study on fracturing of concrete by using SCCD specimens and its potential application in renewable resource energy industry

Author: Xiaoqing Lyu[None]

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The vast utilizing of new resource energy such as solar, wind and nuclear power plant are often together with an shorten tendency of time limit of a project. From the past real cases that can be found that failures produce not only disaster for medical aspects, but also a waste of investor's assets. To prevent all these risks, all of contributors must take care the project in its responsibility. For reduce further threats in a project, a method can be used with careful judgements. Regardless of whether subterranean facilities or structures on the surface are utilized for daily human activities, materials have an indispensable role to play. With the rise in the utilization of artificial materials for underground structures, engineers must be knowledgeable of the dynamics of brittle materials. Moreover, fracturing is a critical failure mechanism of brittle materials and is essential for assessing their performance in underground facilities. Consequently, it is imperative to comprehend crack growth for the purpose of designing safe and secure concrete structures. This research aims to explore the risk awareness of a project in the new resource energy industry by studying the fracture toughness and crack mouth displacement of a concrete specimen to gain an understanding of the crack mechanism. This study employed semi-circular chevron disk (SCCD) specimens with different inclined notch crack angles in order to carry out an experimental investigation. The highest load ever recorded was achieved with a specimen featuring a 60° inclined edge crack. It was observed that the failure load increased with an increase in the notch crack inclination angle. It is plausible to suggest a hypothesis concerning the predictability of fractures under particular circumstances in the renewable energy field.

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Modeling Subsurface Hydrogen Storage With Transport Properties From Entropy Scaling Using the PC-SAFT Equations of State

Authors: Johannes Eller[1]; Tim Sauerborn[1]

Co-authors: Beatrix Becker [1]; Ivan Buntic [1]; Joachim Groß [1]; Rainer Helmig [1]

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Hydrogen is a promising alternative to carbon based energy carriers and may be stored in large quantities in subsurface storage deposits. We investigate the impact of static properties, which are density and phase equilibria, as well as the impact of dynamic properties, being viscosity and diffusion coefficients, on the pressure field during the injection and extraction of hydrogen in the porous subsurface. In a first step, we derive transport properties for water, hydrogen and their mixture using the Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) equation of state in combination with an entropy scaling approach and compare model predictions to alternative models from the literature. Our model compares excellently to experimental transport coefficients and models from literature with a higher number of adjustable parameters, such as GERG2008, while also showing a clear improvement over empirical correlations for transport coefficients of hydrogen. In a second step, we determine the effect of further model reduction by comparing our model against a much simpler model applying empirical transport coefficients from the literature. For this purpose, hydrogen is periodically injected into and extracted out of a dome-shaped porous aquifer under a caprock. Our results show that density and viscosity of hydrogen have the highest impact on the pressure field, and that a representative thermodynamic model is essential for modeling the storage aquifer while keeping the model's number of coefficients at a minimum. In diffusion-dominated settings such as the diffusion of hydrogen through the caprock, our developed diffusion coefficients show a much improved dependence on temperature and pressure, leading to a more accurate approximation of the diffusive fluxes.

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Poster / 330

Spatial microporosity mapping in meso-scale rock samples by X-Ray Computed Tomography

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Porosity is one of the main petrophysical inputs to any reservoir modelling technique, because it affects both the transport and storage properties of the rock. At the laboratory scale, digital rock models can be used to investigate the inner structure of the rock by applying non-invasive X-ray tomographic microscopy. In its most basic application, this approach enables identifying solid material (grains) and void space (pores) from the acquired images. The main limitation of the approach is given by the achievable spatial resolution of the images (voxel size). In the digital rock domain, microporosity is defined as the pore space that is below image resolution –typically established at 1 micron. In carbonate rocks, the fraction of unresolved porosity can be quite large (up to 40%)[1], introducing large uncertainties for the modelling of transport and storage processes.

Here, we propose an image-based experimental workflow to map microporosity in rock cores that uses two distinct X-ray Computed Tomography instruments. For this study, we consider two rock samples, namely Bentheimer sandstone, a homogeneous sedimentary rock with uniform high porosity and essentially no microporosity (Diameter = 1.2 cm, Length = 4.6 cm), and Ketton Limestone, an oolitic carbonate with porosity comprising of intergranular macroporosity and intragranular microporosity (Diameter = 1.2 cm, Length = 3.6 cm). The two instruments used are a benchtop microCT scanner (Bruker skyscan 1273) and a medical-grade CT scanner (TOSHIBA Aquilon 64 TSX-101A clinical X-ray CT) to provide 3D imagery of the same, registered rock sample at (8x8x8) μm3 and (27x27x500) μm3, respectively. The latter defines the maximum resolution at which the proposed workflow can be applied. To this end, a map of the total porosity of the sample (including microporosity) is obtained from differential images by combining dry and water-saturated scans of the rock sample obtained using the medical-grade instrument[2]. This 3D map is then combined with the 3D map of resolved porosity obtained upon segmenting the dry image of the rock sample obtained using the microCT instrument to yield a 3D map of unresolved porosity[3].

Key to the application of the proposed method is the quantification of uncertainties arising from image noise and image analysis (e.g. re-sampling, segmentation) in each step of the workflow. We quantify image noise as a function of voxel size and compute its spatial autocorrelation to identify the minimum voxel size for quantitative analysis. We show that for a medical-grade instrument this can be substantially larger (5-10 times) than the voxel size of the original image. A similar conclusion is drawn for images acquired using the microCT instrument, although in this case a systematic drift of grey-scale values is observed that must be corrected for. We compare results obtained upon application of the full workflow to two rock samples and show that reliable mapping of unresolved porosity (microporosity) must account for these uncertainties. Furthermore, we discuss procedures to minimize uncertainties in the estimated porosity maps (resolved and unresolved) at different spatial resolutions.

Participation:

In-Person

References:

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Poster / 332

Controlling hygrothermics of biobased construction material

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Biobased materials have been applied more and more widely in the field of construction, thanks to their low thermal conductivity and humidity adsorption capacity. The application of them creates a promising way to lower resources assumption and carbon dioxide emission, contributing to sustainable development.
For better application of biobased construction materials, a full understanding of moisture transport process in building envelopes is of vital importance since it can greatly affect the comfort or discomfort that the walls provide to people due to the resulting wetness or heat loss along the walls. Thus, it has an impact on the ventilation and heating demand, which leads to energy consumption reduce. However, our current knowledge of these complex processes is still limited. Factually, the moisture transfer process in the building envelopes is generally not taken into account in the current conventional thermal calculation and energy consumption analysis. The major problem hindering progress is the lack of information and proper description of water transport and phase changes inside the porous structure. Measurements remain challenging, in particular considering that the materials are not transparent and different states of water (free liquid water, bound water, vapor) can coexist. The most difficult point concerns bound water, i.e., water absorbed inside the molecular structure of cell walls, which can hardly be detected with standard imaging.
In this study, we prepare samples made by cotton fibres with varies porosities,
then use them in NMR test, the pores in samples are filled with oil to examine if the bound water

within fibres can be transferred. Following the bound water by NMR, it has been found that there is a network of contacts between the fibers, which allows to transport the bound water throughout the system even when the pores are filled with oil. Then the diffusion coefficient can be measured by analytical solution or finite element method. The diffusion coefficient will vary for different porosities, which can be linked to the variation of compression, leading to the difference of the fibres' orientations. Moreover, letting the diffusion direction being vertical to the compression direction, the value of the longitudinal diffusion coefficient (along fiber axis) can be deduced, and the effect of diffusion direction on the transfer velocity of bound water within fibres can be noticed. Finally, we will consider a model material made by compression of cotton fibres, establish a mathematical model for straightforward analytical predictions of the humidification or drying characteristics of textile materials. Throughout this study, we can get detailed information of the moisture transfer process during drying/humidification process, which can provide insight into the underlying mechanism of the biobased materials, thus paving the way to the application of biobased materials in the field of construction.

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Energy Transition Focused Abstracts:

333

Damage resistance of porous asphalt mixture with additives subjected to freeze-thaw cycles and salt erosion

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In coastal seasonal frozen regions, along with the effects of salt spray, tide and rainfall, salt penetrates the asphalt pavement through porous media. The inner salt will accumulate and deliver, which weakens the cohesiveness of the asphalt-aggregate interface and induces diseases such as spalling and pitting. In addition, the seasonal freeze-thaw cycle causes early damage to the asphalt mixture. Admixture is an effective means to improve the performance of porous asphalt mixture. Efforts done by previous researchers have shown ferrocyanide can inhibit salt crystallization and reduce salt erosion damage of porous materials. Basalt fiber and anti-stripping agent can improve the service performance of porous asphalt mixture. However, the types of three additives have not been applied to freeze-thaw cycles and salt erosion environments, and the specific improvement effect is unclear. Therefore, this paper focuses on porous asphalt mixture damage resistance with additives under freeze-thaw cycles and salt erosion.
Admixtures, including crystallization inhibitor, basalt fiber and anti-spalling agent were chosen to prepare porous asphalt mixture. The samples of porous asphalt mixture with additives were tested for the splitting tensile strength after 15 freeze-thaw cycles and salt erosion. And scanned the characterization of the initial internal structure after 0, 7, 20 freeze-thaw cycles and salt erosion through X-ray computed tomography technology. Changes in strength and internal structure were used to analyze the effect of freeze-thaw cycles and salt erosion action on the porous asphalt mixtures with

additives. On the basis of the internal structure change, the enhancement performance of porous asphalt mixture with additives was evaluated by grey relation analysis and analytic hierarchy process analysis.
Results showed the performance improvement of porous asphalt mixture with crystallization inhibitor is better than anti-stripping agent and basalt fiber asphalt mixture, respectively. The three types of additives only retard the evolution of internal structure and do not change the damaged formation of internal structure inside asphalt mixture under freeze-thaw cycles and salt erosion. Parameters such as air void content, air void number, average void diameter and connective void content have been applied in characterizing the internal structure of porous asphalt mixtures. The internal structure damage dominating causative factors of porous asphalt mixture with additives from large to small are air void number, connective void content, air void content and average void diameter. The internal damage index was introduced to characterize the performance improvement of porous asphalt mixture with additives. The smaller the internal damage index, the better the improvement of porous asphalt mixture. The internal damage index of porous asphalt mixture with crystallization inhibitor is the lowest, which indicates resistance to the action of freeze-thaw cycles and salt erosion is good and suitable for designing asphalt mixtures in coastal seasonal frozen regions.

Participation:

Online

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Energy Transition Focused Abstracts:

Poster / 334

GeoChemFoam, the open-source pore-scale modelling toolbox

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GeoChemFoam is an open-source toolbox for modelling flow processes in porous media images. It is based on OpenFOAM, the open-source Computational Fluid Dynamics (CFD) toolbox, and includes many additional packages that extend the software to more complex physics, including multiphase reactive transport, heat transfer and mineral dissolution, which are essential for modelling porous media applications such as CO2 storage or geothermal energy. Amongst the most popular capabilities of the toolbox is the potential to simulate flow in micro-porous rocks using the multiscale Darcy-Brinkman-Stokes (DBS) model. The objective of the GeoChemFoam project is to support our own research, foster new and existing collaborations, like the ones we currently have with Columbia University and the University of Tohoku, and to provide students around the world with a simulation platform to advance their own research.

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Diagenetic Quantification in Relation to Pore Size Population Using Digital Rock Technology

Authors: NUR SHUHADAH BINTI JAPPERI[1]; KEJIAN WU[2]; ANDREW STARKEY[2]; PANAITESCU CIPRIAN-TEODOR[2]

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Quantifying reservoir property is one of the most crucial works of petroleum exploration and production. Determining transport properties in reservoir rocks requires accurately quantifying the pore system. The study of the pore structure in porous media is to understand the processes of single and multiphase fluid flow. Quantification of the pore system in reservoir rocks at large scale is essential to understand the displacement process in the field to locate the remaining hydrocarbon. To acquire a better understanding of the diagenesis of reservoir rock and pore structure, a quantitative method is required. In principle, a representative large-scale multiscale pore structure model for heterogeneous reservoirs can be constructed by adding diagenesis and facies in the reservoir modelling. This study tries to use the detailed pore structure and diagenesis information from high-resolution scanning electron microscopy (SEM) imaging to quantify the diagenesis linked to the reservoir rocks' quality. This involves the quantification of population of pore and grain size distribution and cement spatial distribution features of rock samples by categorising them into three different classes. The North Sea Oil Field data is used as a case study.

Based on the cement feature segmented from high-resolution SEM image, the limit of segmentation of cement, the connectivity of cement particle was observed and evaluated. Through the pore size distribution functions fitting, the cubic polynomial exhibits the best fits for pore population from the North Sea Oil Field data. The digital rock tools are able to provide the details of the pore structure and associated diagenetic process with lithofacies. The quantitative results can be used for further analysis on diagenesis process that can be then linked with well logging features at next study.

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Microscopic flow parameters prediction of shale oil based on deep learning

Authors: Liang Zhou[None]; Hai Sun[None]; Lei Zhang[None]; Yongfei Yang[None]; Jun Yao[None]

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Abstract:Shale oil is a valuable unconventional oil and gas resource. It has a complex mineral composition, and rapid and accurate prediction of core flow parameters is crucial for its exploration and development strategy. At present, researchers predict flow parameters such as speed,pressure,apparent permeability,etc. through core experiments that require specific experimental conditions and methods, which are difficult and time-consuming. Conventional simulation methods for predicting flow parameters require considerable computational resources. Therefore, deep learning can be used as a pore-scale simulation prediction method. Considering that the mineral properties of the nanopore wall of shale oil have a large influence on the flow, a core dataset with organic distribution.
We predict the flow parameters of shale oil porous media by two methods. First,we designed a convolutional network for the dataset, adopted the structure of SE-ResNet, added the squeeze-and-excitation (SE) module to the double-layer residual module of ResNet18, and combined the characteristics of the SE block with the attention mechanism and ResNet to effectively obtain the information between channels and avoid the problem of gradient disappearance or explosion. Using SE-ResNet for directly predicting the apparent permeability from images. Another method attempts to couple a point cloud residual network with flow equations, reconstruct the flow field and predict apparent permeability. The coordinates of the porous media pore space are used as input to the point cloud network. Different slip conditions are set for organic and inorganic matter. The loss function of the neural network is constructed by the NS equation, the continuity equation, and the flow boundary between organic matter and inorganic matter.Based on the principle of PINN, optimization algorithms such as gradient descent are used to obtain the weight parameters of neural network connection and the physical parameters of partial differential equations. Only sparse data acquisition points are required to predict microscopic flow parameters. The above two methods are well applied in shale porous media.

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Pore-scale simulation of acidic dissolution in porous media with sub-resolution porosity using the improved multiphase micro-continuum approach

Authors: Zhiying Liu[None]; Qianghui Xu[None]; Junyu Yang[None]; Lin Shi[None]

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The chemical dissolution of carbonate rocks occurs in multiple natural and industrial processes, such as the acidizing stimulation of petroleum reservoirs and the geologic carbon sequestration. The dissolution dynamic involves multiscale porous structures and complex interactions of multiphase flow, interfacial mass transfer and heterogenous reactions across various length scales, which is necessary to advance the mechanistic understanding from the pore-level simulation. The micro-continuum approach can perform direct numerical simulations of reactive flow in porous samples containing sub-resolution porosity and avoids mesh dynamic updates during the dissolution process. However, unacceptable spurious velocities often appear near the gas-liquid interface and the three-phase contact line region, which limits the use of the micro-continuum approach in capillary-dominated multiphase reactive flows. In this study, the micro-continuum approach is improved to reduce the spurious velocities in the simulation of capillary-dominated flow and more accurately predict the transport and reaction processes. The improved method is validated by a series of static and dynamic benchmark cases to demonstrate that the improved micro-continuum model can simulate capillary-dominated multiphase flows with negligible spurious velocities at capillary numbers as low as 10-4 in both simple and complex geometries, 1-2 orders of magnitude lower than the previous micro-continuum method. As to the interfacial mass transfer, the compressed continuum species transfer model is introduced to reduce the artificial mass transfer in the gas-liquid interface. The effects of sub-resolution porosity and gas/water distribution on dissolution dynamics are investigated for different dissolution patterns. The numerical results show that the sub-resolution porosity significantly impacted the flow, transport, and dissolution processes in heterogeneous porous media.

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MS06-A / 339

Analytical and numerical investigations of imbibition in porous media

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The multiphase flow of fluids in a porous media is attributed to viscous, gravitational and capillary forces. A theory was proposed by Buckley and Leverett for viscous dominated flow during the last century which is used to estimate the rate at which the injected water moves through a porous medium. In this work, we study and investigate the phenomenon of imbibition which is the taking

up of a wetting liquid by a porous solid. We present analytical and numerical solutions for spontaneous imbibition in one dimension by the use of fractional flow theory. The solutions can also be understood as the capillary analog to the classical Buckley Leverett solution and are valid for co-current displacement, with arbitrary fluid viscosities, as well as for capillary pressure and relative permeability curves dependent on saturation. We measure the saturation profiles as a function of distance and time in fluid-filled porous media with some initial wetting fluid saturation. We create a 1-D model on a numerical simulator to simulate and obtain saturation profiles for the different wettability cases assuming horizontal immiscible displacement in porous media. We then match simulation results with saturation profiles obtained through the capillary dominated flow semi-analytical solution proposed in literature. The solution can be used to study the influence of wettability, predicting saturation profiles and production rate characteristics.

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Energy Transition Focused Abstracts:

Poster / 340

Assessing formation damage in-situ using X-ray computed tomography

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The flow of sub-surface suspensions, and the controls on mobilisation, transport and deposition of a suspended load are important in natural (ground water migration, hydrocarbon migration, pollutant transport) and industrial (nuclear waste storage, CCS, hydrocarbon recovery) applications. In all of these areas we seek to understand how and when a suspended load moving through porous media will be deposited at pore throats; and how this can change permeability, flow pathways, and ultimately prevent further fluid migration. The inherent complexity of pore networks makes particle migration difficult to predict. Formation damage describes processes of deposition from a suspended load that reduce the permeability and porosity of a host rock. The processes that lead to formation damage are challenging to quantify because of the dynamics and opaqueness of host systems, requiring pore scale processes to be studied via bulk measurements of inlet/outlet pressure and particle concentration measurements. Formation damage commonly occurs during subsurface drilling, due to the drilling fluid changing system chemistry which liberates host rock particles and acts as a source for a relatively high-volume fraction suspended load. We use bespoke in situ flow cells with a combination of high speed x-ray radiography and x-ray computed tomography to image and quantify how particles suspended in a single-phase fluid behave in real time. We show how and where mobilisation, transportation, and deposition from the suspension occurs, how they are related to flow rates, particle volume fraction, and the (evolving) local pore-network geometry. We

also compare the observed behaviours to CFD simulations through the same pore network to verify the simulations accuracy. This information can then be used to make informed decisions when choosing drilling fluid constituents to limit formation damage. In the future we aim to observe how salinity and pH impacts formation damage processes.

Participation:

In-Person

References:

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MS12 / 341

Coupling mechanism of sorption and deformation in amorphous cellulose with hierarchical porous structure

Authors: Lingji Hua[1]; Ali Shomali[None]; Chi Zhang[None]; Dominique Derome[2]; Jan Carmeliet[3]

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Wood, as natural adsorbent and significant building material, features complex biopolymer composition and hierarchical porous structure, endowing it with distinguished sorption properties accompanied by sorption-induced deformation. In former studies, sorption, deformation and sorption-deformation interactions have been studied for single-scale materials, but not for materials where micropores and mesopores coexist. This work, establishing a mesoscopic slit pore between two slabs of amorphous cellulose with micropores, aims to provide a first attempt at modeling sorption and sorption-induced deformation in hierarchical porous structure. Specifically, the atomic system is numerically modeled by a hybrid workflow synthesizing molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) simulation. Based on the simulation, sorption/deformation mechanisms in porous materials with different slit size are clarified. In microscopic pores prevailing in the cellulose slab, pore filling happens throughout the full relative humidity (RH) range. Under low RH, adsorption happens mainly by filling existing voids. At high RH, adsorption continues via imposing a sorption stress, leading to a swelling and additional sorption of the microporous material. In the mesoscopic slit pore between the two cellulose slabs, surface sorption takes place, with negligible amount initially but remarkable thickness with increasing RH. Meanwhile, increasing surface roughness is observed, in response to the varying surface energy caused by the multilayer adsorption. At a certain RH, the water molecules residing on the opposite cellulose slabs undergo capillary condensation, which exerts a negative hydrostatic pressure perpendicular to the slab surface on the

structure, resulting in an increase in slab volume, a decrease in distance between the center of mass (COM) of the slabs and thus a thinning of the slit pore.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 342

Influence of phototrophic biofilms on nutrient availability in soil

Author: Jonas Kollmen[1]

Co-authors: Katharina Wastian [1]; Dorina Strieth [1]

[1] *RPTU Kaiserslautern-Landau, Chair of Bioprocess Engineering*

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In the current times, the protection of the environment is becoming more and more important in all sectors. This also includes agriculture, which has to overcome particularly large hurdles in this respect, since on the one hand the world population is steadily increasing and thus more people have to be fed, but on the other hand the usable land is limited. Therefore, the yield must be increased, which is mainly done through the excessive use of mineral fertilizers, which are extremely energy-intensive to produce and are harmful to the environment. Therefore, natural, living fertilizers are searched that form a mutualism with crop plants. Thus, the problems of over-fertilization can be overcome. Cyanobacteria, ubiquitous phototrophic prokaryotes, are a possible source of biological fertilizer, mainly because of their ability to fix elemental nitrogen from the atmosphere and to release it in a usable form into the environment. Among other organisms, cyanobacteria are able to enter into symbiosis with plants, whereby not only nitrogen but also other nutrients or growth-promoting substances can be exchanged. Furthermore, cyanobacterial biofilms contribute to an improvement of the soil condition. By producing extracellular polymeric substances, which consist largely of polysaccharides, it can positively influence both soil aggregation and soil water retention and thus reduce soil erosion. In addition, the biofilm can also change the nutrient composition or availability in soils. Cyanobacteria thus represent a promising environmentally friendly alternative to traditional fertilizers.
Wheat is one of the most important food grains in the world, so this work investigates the co-cultivation of common wheat (*Triticum aestivum*) and cyanobacteria. Diazotrophic strains isolated from the temperate zone are used as cyanobacteria to investigate the effect of nitrogen fertilization by cyanobacteria on the growth of wheat. In addition, the influence on nutrient availability will be investigated by analyzing the pore water. Furthermore, it will be determined whether the use of cyanobacteria can lead to an increase in water retention in the soil. All experiments are conducted in typical agricultural soils for a complete growing season of wheat.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-A / 343

ET-MIP: A coupled model approach to simulating the fate and transport of CO2 in overburden

Author: Nicholas Ashmore[1]

Co-authors: Ian Molnar [1]; Stuart Gilfillan [1]; Magdalena Krol [2]

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Carbon capture and storage (CCS) has emerged as a principal emissions reduction technology for the energy transition. Its effectiveness hinges largely on the security of the storage reservoir, which may be susceptible to leakage through permeable pathways such as abandoned wells and faults. Storage failure presents risks of environmental impacts, increases atmospheric carbon emissions, reduces the value of carbon credits, and reduces public confidence in CCS as a viable technology for the energy transition. Despite the importance of storage security, our understanding of CO2 leakage and its fate and transport in overburden remains limited, hindering the prediction, detection and assessment of leaks. There is a need for numerical models capable of accurately predicting the fate and transport of CO2 in the subsurface. However, traditional multiphase flow models struggle to describe the buoyant unstable gas flow regime expected at leak sites, motivating the use of other modelling approaches.

Unstable gas flow is characterized by discontinuous gas clusters and sharp variations in gas saturations in space, in contrast with the smooth variation in gas saturation predicted by continuum multiphase flow models. Discrete approaches such as macroscopic invasion percolation are better equipped to model unstable gas flow and are less computationally intensive, however they are limited by assumptions of instantaneous gas movement. ET-MIP (Electro-thermal macroscopic invasion percolation) is a general purpose model which couples continuum-based electrical, thermal, groundwater and chemical species modules with a discrete macroscopic invasion percolation gas flow module. This coupled approach allows for accurate simulation of slow gas displacement characteristic of shallow subsurface gas releases while simultaneously predicting the dissolution of CO2. ET-MIP has been validated against bench scale experiments and shown to accurately predict gas generation, multiphase transport and capillary trapping –all mechanisms which govern the fate of CO2 in the subsurface. However, the model has not yet been applied to gas injections with simultaneous mass transport. This talk will present validation of ET-MIP against a bench-scale CO2 injection and dissolution experiment, and explore the migration of leaking CO2 in the subsurface.

Participation:

In-Person

References:

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MS15 / **344**

Physical residual neural networks for reduced order modelling of reactive flow in porous media

Authors: Ahmed H. Elsheikh[1]; Hannah Menke[1]; Julien Maes[1]

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Accurate prediction of solid mineral dissolution during reactive flow in porous media is vital for a wide range of subsurface applications (e.g., CO2 sequestration [1] and geothermal systems [2]). Detailed numerical modelling of mineral dissolution at the pore-scale is generally expensive [3] and that limits our ability to perform comprehensive uncertainty quantification studies to explore the various sources of uncertainties and its impact on the dissolution process.

In this work, we develop efficient deep learning emulators for geochemical reactions. We build on an earlier work on reduced order modelling (ROM) using Deep residual recurrent neural network [4] to develop highly predictive ROM using limited training data. We utilize a U-net architecture to perform approximate explicit time stepping for the dynamical system. The input features for the deep learning model are the discrete components of the physical residual which are known to correlate well with the solution updates over the training samples as well as the unseen validation dataset. This correlation is governed by the physical equations controlling the evolution of the system. The second component of the DL emulator is a hierarchical architecture of neural networks, where a stack of U-Nets is used at every timestep to mimic fixed point iterations in numerical schemes. In order to stabilize the training, the algorithm starts with a single step update, after which, the first level U-Nets are frozen, and the next level U-Net is trained and so on.

The developed algorithm is demonstrated on a dataset with different Peclet and Kinetic numbers. The pore-scale dissolution training and validation datasets are generated using detailed numerical simulations using the improved Volume-of-Solid method in GeoChemFoam [3] and are available as an open access repository for a range of dissolution regimes [5].

Participation:

In-Person

References:

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MS14 / 345

Roles of Transport Mechanisms and Model Parameters in Gas Flow Migration across low-permeability porous media

Authors: Leonardo Sandoval[1]; Alberto Guadagnini[1]; Monica Riva[1]; Ivo Colombo[2]

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[2] *Geolog International*

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Appropriate modeling approaches to quantify gas migration in low-permeability porous media can assist appraisal of sealing efficiency of caprocks, with key applications in sustainable use of underground energy resources. A variety of models depicting gas movement across low-permeability geomaterials are available (Wu et al., 2016; Sun et al., 2017, Rani et al., 2018). Some of these models represent gas migration in low-permeability media as a weighted sum of diverse mechanisms taking place across the porous system. Parameters associated with these models are envisioned to embed the chemical, mechanical, flow, and transport features governing feedbacks between gas and the host rock matrix. Such parameters cannot be easily and unambiguously evaluated via experimental investigations and are always affected by uncertainty. In this context, modern sensitivity analysis techniques enable us to diagnose the behavior of a given model through quantification of the importance and role of model parameter uncertainties onto a target model output.

Here, we rely on two global sensitivity analysis approaches and metrics (i.e., variance-based Sobol' indices and moment-based AMA indices) to assess the behavior of a recent interpretive model that conceptualizes gas migration as the sum of a surface diffusion mechanism and two weighted bulk flow components (i.e., Slip flow and Knudsen diffusion). We quantitatively investigate the impact of each uncertain model parameter on the evaluation of methane flow, which is, in turn, conceptualized as a random quantity. Considering the paucity of available information, we consider three diverse characterizations of the probability density function describing the uncertain model parameters: (**a**) all parameters are described by uniform distributions; (**b**) all parameters are represented through truncated normal distributions; and (**c**) the reference pore radius is described by a truncated log-normal distribution while the remaining parameters are associated with uniform distributions. We then derive analytically the structure of an effective diffusion coefficient embedding all complex mechanisms of the model considered and rely on the global sensitivity analysis results to quantify the relative contribution of each flow mechanism to the overall gas flow.

Our results suggest that, in decreasing order of importance, reference pore radius, reference porosity, pore pressure, tortuosity, and temperature are the model parameters driving the major features of the gas flow probability density function. These results remain essentially unaffected by the choice of probability density function characterizing model uncertain parameters.

Participation:

In-Person

References:

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346

Adsorption and Oversolubility in Hierarchical Nanoporous Zeolites

Author: Vishnu Prasad Kurupath[1]

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Adsorption inside nanoporous materials has driven large scientific interest due to their key-role in numerous applications such as in catalysis, adsorption/separation, etc. [3]. Among nanoporous materials, hierarchical solids are an interesting class in which nanopores ranging from micropores, mesopores, and macropores are arranged in a continuous fashion [8]. As a result, these hierarchical nanoporous materials possess enhanced combined adsorption/transport capabilities as larger pores provide pathway towards smaller adsorption sites. Further, owing to the presence of different pore sizes, hierarchical nanoporous materials are also useful for size selective applications [9]. For example, hollow zeolite shells made by imposing mesoporous cavities over the inherently nanoporous zeolitic lattice show capacity for size selective catalysis, adsorption and transport [1]. While zeolitic materials are widely studied for adsorption/catalyis applications, the influence of large external surface areas and the resulting interfaces in hierarchical zeolites have not been widely explored [7, 4]. Further, gas solubility inside confined liquid solvents are often larger than bulk systems [6, 5]. This phenomena is recognized as oversolubility (liquid-gas mixtures) or preferential adsorption (gas-gas mixtures) and is never explored comprehensively [2].

Here, we report adsorption in hierarchical zeolites obtained using Grand Canonical Monte Carlo (GCMC) simulations. Studies on both bulk zeolite lattice and bi-porous zeolite system are discussed with focus on bulk and surface adsorption. Pure gas binary mixtures of toluene, ethylene and water were tested for adsorption and gas solubility in liquid toluene and liquid water inside the zeolite was quantified. The adsorption thermodynamics of the gas mixtures and the liquid-gas solution are obtained. Further, preferential adsorption of the gas phase species and gas oversolubility in liquid

solvent under confinement is also explored. The impact of surface on adsorption and the surface adsorption characteristics are quantified and adsorption characteristics inside bi-porous zeolites with water only present at the outer surface is also discussed.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS06-B / 347

Deformation-driven collapse of gas cavities in a soft porous medium

Author: Oliver Paulin[1]

Co-authors: Liam Morrow [1]; Matthew Hennessy [2]; Chris MacMinn [1]

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Gas bubbles can form and grow in otherwise liquid-saturated granular media due to various physical processes, such as corrosion or the microbial decomposition of organic matter. These gas bubbles are typically non-wetting to the solid grains; as such, it is energetically costly for the gas to invade the narrow pore throats between grains. If the solid skeleton is sufficiently soft and/or the confining stress is sufficiently low, the gas can instead displace the solid grains to open macroscopic cavities. These gas cavities form in a variety of soft porous media, including seabed sediments, industrial waste ponds, and peatlands. An increase in the confining stress can trigger the collapse of these cavities, forcing the gas into the pore space. A quantitative understanding of cavity collapse is thus important for characterising the macroscopic mechanics of this three-phase system and for predicting the rate of gas venting to the surrounding environment. Here, we investigate this problem experimentally using a packing of hydrogel beads as a model soft porous medium. We complement our experimental observations with a novel phase-field model that captures the competing effects of elasticity and gas-liquid-solid interactions (capillarity). We study the deformation-driven collapse of gas cavities in a 1D setting, identifying the confining stress at which cavities collapse and investigating the reversibility of cavity formation and collapse under fluctuating confining stress.

Participation:

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References:

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Energy Transition Focused Abstracts:

Poster / 348

Simulation of transition flows and phase changes in porous media using modified equations of state to obtain the correct surface tension

Author: Javier Fernández-Fidalgo[1]

Co-authors: Luis Cueto-Felgueroso [2]; Luis Ramírez [3]; Abel Martínez [4]; Xesús Nogueira [3]

[1] *Universidade da Coruña and Universidad Politécnica de Madrid*

[2] *Universidad Politecnica de Madrid*

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The phenomena of phase change and coexistence of two phases of a substance are of great interest in engineering. The two most widespread ways of describing these phenomena numerically are the sharp interface [1] and phase field [2] numerical models. The former assume that there is an abrupt transition at the interface between the two fluid phases while the latter propose a smooth transition with a thickness greater than zero. The latter approach takes advantage of the same equation of state (EoS) to describe the thermodynamic properties of both phases. The most widely used EoS, the Van der Waals EoS [3], while obtaining reasonable results for a wide set of substances, in the case of water is quite far from the experimental results. The major current challenge for the simulation

of multiphase and multicomponent pore-scale flow in permeable media is the effect that EoS has on the effective surface tension. In the present work it is shown that multiphase flow simulations based on traditional equations of state (e.g. cubic EoS) result in surface stresses that are several orders of magnitude larger than the actual ones, when intended to simulate problems of interest in geosciences and engineering where the characteristic length of the problem is much larger than the physical width of the interface (on the order of nm). A modification of the Van der Waals EoS is proposed by applying the methodology proposed in [4] with applications to numerical modeling of phase changes in porous media.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS22 / 349

Towards multiphase transport layers - Binary pore size distributions with hydrogen bubble assisted electrodeposition

Author: Adrian Mularczyk[1]

Co-authors: Daniel Niblett ; Adam Wijpkema [1]; Martin de Waal [1]; Marc van Maris [1]; Antoni Forner-Cuenca [2]

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In electrochemical devices, porous transport layers (PTLs) bridge the gap between flow fields and catalyst layers. They provide pathways for liquids and gases to be distributed over and removed from the catalyst layer, provide mechanical support as well has thermal and electrical conductivity. As the electrical current drawn from such devices is directly linked to the flow of reactants, the mass transport capabilities of the PTLs become especially critical at high current density operation. State of the art PTLs are primarily fiber-based (e.g. carbon, titanium) as they satisfy the complex requirements posed by their operating environment. However, in two phase counter flow operation, undesirable liquid accumulations and subsequent blockage of gas transport pathways can occur. Excessive accumulations of reaction products or a lack of fresh reagents stall out the electrochemical conversion, limiting the achievable power density. To overcome these limitations, alterations and improvements to the base material have been investigated to guide liquids and gases into dedicated pathways within the porous structure[1–4]. While they show varying degrees of success, they require additional processing steps, adding cost, and are still limited by both phases having to compete for the same pore network.

We explore the synthesis of hierarchical PTLs containing dedicated pathways for the transport of liquid and gas, realized by a difference in pore sizes on two distinct length scales. While 3D printing is positioned as a promising manufacturing route, currently this method lacks the production speed and resolution. Therefore our approach is focused on an alternative synthesis route whereby the porous material is generated by co-depositing a metal and a gas from a solution containing the metal salt and a source of protons to form hydrogen gas. The hydrogen acts as dynamic template which, together with the deposition kinetics of metal at high overpotentials, forms a structure containing macroscopic and microscopic pores (Figure 1a). This type of structure has in the past been used successfully to improve boiling heat transfer[5], and has been postulated to find application in other electrochemical devices such as batteries or fuel cells[6].
In this talk, I will discuss the necessary development steps to adapt this material for the use in electrochemical systems. At the core of the synthesis route we conceptualized an approach to manufacture self-standing PTLs from this material while preserving its hierarchical microstructure. This enables its use as transport layer and allowed for the application of a wide range of characterization methods to link the synthesis parameters to the resulting material microstructure. Structural information (Figure 1b) obtained through X-ray tomographic microscopy was used to perform transport simulations and ascertain the potential of the material as PTL. The simulations showed increased diffusive transport in dry and liquid filled state compared to state-of-the-art materials. Through careful tuning of synthesis parameters and post treatment steps, the mechanical stability was improved substantially to the point where the integration in electrochemical systems is possible. If successful, this could open the door to a new class of PTLs tailored to the transport requirements of a given system.

Participation:

In-Person

References:

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Poster / 350

Electrode Design Booster Using a Statistical Digital Twin

Author: Mathias Fingerle-Straß[1]

Co-authors: Ilona Glatt [1]; Fabian Biebl [1]; Erik Glatt [1]; Janine Hilden [1]; Sarah Reeb [1]; Roman Buchheit [1]; Andreas Wiegmann [1]

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Highly performing Li-ion batteries are needed as part of reliable energy storage systems to successfully master the transition to renewable energies. To meet this challenge, batteries must be fast-charging, long-lasting, sustainable, and cost-effective to manufacture, while also offering high storage capacity. One essential piece of this highly challenging puzzle resides in improving the microstructure of the electrodes, i.e., on a length scale of a few nanometers to a few hundred micrometers.

The use of direct experimental approaches is difficult at this scale - even sometimes impossible – and also expensive and time-consuming. Alternatively, running simulations to specifically improve batteries at these scales is extremely useful. Simulations provide data to be used as reference for the microstructure of the electrode and help to determine the critical parameters for performance improvement. Our work is carried out on a complete commercial software environment called GeoDict, which is suitable to perform all necessary steps.

A starting point to improve the microstructure is to reliably reproduce the original material with a model. We call this model a statistical digital twin when the performance parameters match those of the original material, and at the same time the geometric properties on the micro-scale match those of the original material in a statistical sense.

This talk will show how to create a digital twin of an electrode material. Starting from a microCT scan, all steps up to the validation of the resulting properties will be explained.

All starts with an image stack of an anode material and performing image processing to improve image quality. Then, the material phases are segmented and the 3D structure is reconstructed. Subsequently, the statistical properties of this imported 3D structure are calculated, such as open and closed porosity, tortuosity, or diffusivity. Using this data and starting from grains with a certain shape and size distribution, the volume fraction of these grains is determined and their shape is adjusted to create an statistical digital twin of the original 3D structure. Finally, the binder-carbon black (CBD) is added at a certain contact angle to the structure.

The resulting statistical digital twin is validated by comparing its porosity, tortuosity, and diffusivity to the same parameters of the originally imported 3D structure. To finely adjust the result, an automatic structure generation iteration may be scripted using GeoPy, the Python interface in GeoDict.

As application example, we show a case study that displays how batteries may be improved by 3D microstructuring approaches. We simulate the structuring of a graphite anode with a laser and describe how these changes affect crucial parameters of the material, such as tortuosity and diffusivity. This work was performed during the structur.e project of the BMWK [1]. In this project, laser perforated electrodes are manufactured and studied experimentally and via simulations to elaborate design principles for fast-charging anodes. Additionally, this project tested alternative design options, like laser ablation of the CBD-phase and using a graded grain size distribution in the electrode.

Participation:

In-Person

References:

[1] https://math2market.com/math2market/publicly-funded-projects/structur-e.html

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Poster / 351

Dynamic pore network modeling of imbibition in porous media with corner film flow

Authors: Jianlin Zhao[1]; Guangqing Zhang[1]; Qinjun Kang[2]; Dominique Derome[3]; Jan Carmeliet[4]

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[2] *Los Alamos National Laboratory*

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Wetting film can develop in the corners of pore structures during imbibition in a strongly wetting porous material, which may significantly influence the two-phase flow dynamics. Due to the large scale difference between main meniscus and corner film, accurate and efficient modeling of the dynamics of corner film remains elusive. In this presentation, we develop a novel two-pressure dynamic pore network model incorporating the interacting capillary bundle model to analyze the competition between main meniscus and corner film flow in real porous media. A pore network with star-shaped pores and throats is extracted from the real porous material based on the shape factor and cross-sectional area, which is then decomposed into several layers of sub-pore-networks, where the first layer of sub-pore-network simulates the main meniscus flow while the higher layers characterize the corner film flow. The flow conductance of throats in different layers of sub-pore-networks are determined by high-resolution two-phase lattice Boltzmann modeling, thus inherently consider the viscous coupling effect. In addition, the snap off mechanism is incorporated which may play an important role under low flow rate condition. The accuracy of the developed dynamic pore network model is validated with both lattice Boltzmann simulation of imbibition in a strongly wetting square tube and microfluidic experiments of imbibition in a strongly wetting real porous chip. Then the model is used to simulate imbibition in a strongly wetting sandstone porous medium and the competition between main meniscus and corner film flow is analyzed. With the increase of capillary number (flow rate) and viscosity ratio between wetting and non-wetting fluids, the development of wetting corner film becomes less significant. Based on these two parameters, a phase diagram characterizing the competition between main meniscus and corner film flow is proposed, which may shed light to the design of some porous media related engineering processes, such as geological CO2 storage.

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Energy Transition Focused Abstracts:

MS22 / 352

Scan Line Patterning: An Efficient Approach to Achieve Periodic Open Cell Structures in Selective Laser Melting

Authors: Alexander Limper[1]; Anselm Brodersen[1]; Matthias Wessling[2]; John Linkhorst[3]

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The adaptation of additive manufacturing for chemical flow reactors has recently gained momentum as the manufacturing methods become more advanced and manufacturing equipment is increasingly affordable.[1] Periodic open cellular structures (POCS) from additive manufacturing have lately received growing attention. Compared to randomly structured substrates such as metal foams, POCS offer an ordered structure, which promises improved flow control and homogeneous flow profiles at comparably low pressure losses. However, the achievable minimum cell size is still limited to few millimeters, which results in low specific surface areas compared to conventional metal foams.[2] Moreover, finely-resolved 3D models that define these POCS require an extensive amount of computing power with increasing resolution and corresponding large file sizes. A scale-up to industry-relevant sizes is therefore limited. Consequently, the direct definition of micro-features in large 3D models is infeasible, as STL files that directly define POCS will reach gigabyte sizes for reactors with outer dimensions of few centimeters and with POCS cell sizes of few millimeters and strut sizes in the millimeter range.

We have recently shown that the porosity and thus the specific surface area in selective laser melting (SLM) can be globally controlled via the laser energy density.[3] In this work, we now present a method to create defined microfeatures, without the need to explicitly define the features in a CAD model, thus avoiding large file sizes. Our method requires no definition of micro-features in 3D models such as STL files, but rather makes use of the scan lines, i.e., the path with which the laser proceeds through the powder bed. By actively controlling the scan line pattern of each layer, repeating structures are created implicitly. The scan line pattern is defined in the print job file, requiring only a 3D model of the macrostructure, which may be as simple as a cylinder, thus only amounting to a file size of few kilobytes.

As example for the simplest form of POCS, a cubic structure is created with cell sizes as small as 400 µm and strut thicknesses of approximately 100 µm. The resulting structures are analyzed by reconstruction of 3D models from micro-computed X-ray tomography.[4] From the model, the strut thickness, cell size and specific surface area can be derived, which presents as beneficial compared to other imaging methods such as SEM, where the analysis is limited to the surface.

Figure 1 presents a model POCS structure, consisting of cubic cells with a cell size of 800 µm. The strut sizes and specific surface area are approximately 120 µm and 5.6 x 10^3 m^2/m^3, respectively, which is well in the range of commercial metal foams.

The presented method therefore shows great promise to propel the design of highly active, open-porous reactor systems to industrially relevant scales with small feature sizes that have sparsely been reported in literature so far.

Participation:

In-Person

References:

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MS17 / **353**

Investigation on the impact of thermo-osmosis on fluid pressurisation in Boom clay –a case study of the ATLAS in-situ full-scale heating experiment.

Authors: Feliks Kiszkurno[1]; Thomas Nagel[2]; Jörg Buchwald[3]; Olaf Kolditz[4]

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[2] *Technische Universität Bergakademie Freiberg, Germany*

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Existing literature suggests the importance of the thermo-osmosis (TO) for an accurate simulation of pore pressure evolution in heater tests for nuclear waste disposal in clay rock. However, there is limited consensus regarding the appropriate choice of parameters controlling TO and the extent of its physical impact. This study will use the ATLAS in-situ heating experiment, a full-scale experiment from an underground research laboratory in Mol in Belgium, to investigate the impact of TO on the thermal pressurisation in Boom Clay.
The ATLAS experiment was simulated using the open-source code OpenGeoSys. A fully coupled thermo-hydro-mechanical model combined with an inelastic constitutive model for the host rock was used. After comparison to published data, a parameter study, using an Assisted-History-Matching workflow (Buchwald et al., 2020), was performed to obtain a good representation of the in-situ measurements without taking into account TO. Next, the same procedure was repeated with a model extended to account for TO. The comparison of both groups allows a clearer discussion of the influence of TO on temperature and pressure evolution in the studied system. The final step - uncertainty quantification of the TO parameterisation, puts the results in the context of large uncertainty of parameters documented in the literature. The impact of the said uncertainty will be illustrated by a range of plausible model predictions.

Participation:

In-Person

References:

Buchwald, J., Chaudhry, A. A., Yoshioka, K., Kolditz, O., Attinger, S., & Nagel, T. (2020). DoE-based history matching for probabilistic uncertainty quantification of thermo-hydro-mechanical processes around heat sources in clay rocks. International Journal of Rock Mechanics and Mining Sciences, 134(September). https://doi.org/10.1016/j.ijrmms.2020.104481

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Poster / 354

Predictive Digital Rock Physics simulation applied on a Sandstone Reservoir

Authors: Mohamed Regaieg[1]; Titly Farhana Faisal[1]; Franck Nono[2]; Cyril Caubit[1]

[1] *TotalEnergies OneTech*

[2] *Modis*

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Digital Rock Physics (DRP) simulation provides a fast and cheap way to compute relative permeability curves of a rock/fluids system. It represents an opportunity to provide more data to Reservoir engineers and thus help them to have better petrophysical input for their simulations. In a previous work, we have shown that DRP simulation was predictive for a mixed-wet Bentheimer when coupled with a wettability anchoring experiment (Regaieg et al 2022). In this work, we first apply TotalEnergies DRP simulation workflow in an operational context on Reservoir sandstone sample while coupling it with a wettability anchoring experiment. Images representing large volumes with low resolution are, first, improved with Enhanced Super Resolution Generative Adversarial Networks (ESRGAN) in order to obtain a large images with high resolution. Then, a pore network is extracted and TotalEnergies parallel pore network simulator is used for multiphase flow simulations taking into account the constraints from the anchoring experiment to include wettability information. Subsequently, we compare the results against an in-house SCAL experiment. This allows us to assess the predictive power of our DRP workflow on a sandstone Reservoir rock. After that, new simulations are performed using a new sample from the same facies without carrying out a new anchoring experiment. Finally, the simulation results are compared to a second in-house SCAL experiment and the extrapolation power of DRP simulation is assessed.

Participation:

In-Person

References:

Regaieg, M., Nono, F., Faisal, T. F., & Rivenq, R. (2022). Large Pore Network simulations coupled with innovative wettability anchoring experiment to predict relative permeability of a mixed-wet rock. Research Square. https://doi.org/10.21203/rs.3.rs-1878809/v1

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Poster / 355

Biomineralisation of Calcium Carbonate via Ureolytically Active Fungi

Author: Jason Eriksen[1]

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Over the last 15 years there has been increasing interest in the use of microbially-induced biomineralisation processes for a range of civil, structural and environmental engineering applications including for rock fracture grouting, soil stabilisation, well sealing, stone and concrete protection/repair and bioremediation. Most studies have focused on investigating calcium carbonate precipitation via ureolysis using bacteria, with very few studies investigating other microbes. However, fungi are also known to induce biomineralisation extensively in the natural environment. One potential advantage of using filamentous fungi over bacterial-based systems is the ability for fungi to grow in situ within porous media. Filamentous fungi grow as hyphae that extend, branch out and fuse back together as the organism searches for nutrients within a porous media, forming a 3D network called the mycelium, which can subsequently be used as a scaffold for mineral precipitation. The overall aims of this research are to (i) identify ureolytically active fungal species which can contribute to calcium carbonate precipitation and (ii) develop treatment strategies for stabilising sands using fungal-induced biomineralisation.

An experimental screening programme was carried out using five basidiomycota fungal species native to the UK: *Lyophyllum decastes*, *Lepista nuda*, *Pleurotus cornucopiae*, *Pleurotus ostreatus*, and *Pleurotus pulmonarius*. Screening was focused on assessing: (i) growth rate via time lapse photography and (ii) urease activity using a phenol red assay and monitoring of NH4+ production and Ca2+ depletion in batch experiments. *Pleurotus cornucopiae* was identified as being the fastest growing and most ureolytically active of the fungal species screened.

Pleurotus cornucopiae was taken forward to the second stage of the research and the conditions required for growth within sand columns was investigated. Factors considered included time for growth of fungal inoculant within broth, growth time within sand column, media grain size, carbon source, and grain size of carbon source. The treatment methodology has also been investigated with the goal of achieving mechanical strength improvement. Variables investigated include concentration of cementation solution, cycle duration, number of cycles and injection strategies. The influence of these variables on mass of calcium carbonate was determined and optical and scanning electron microscopy conducted to investigate crystal morphology and mineral distribution within the porous media. These results demonstrate that improvement in the mechanical behaviour is governed by not only the distribution of calcium carbonate within a treated medium but also the nature of the crystals formed via fungal biomineralisation.

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In-Person

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Energy Transition Focused Abstracts:

MS01 / 356

he moisture and temperature evolution in a zeolite heat storage reactor during cycling: an NMR study

Author: Leo Pel[1]

Co-author: Jelle Houben [1]

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Society is focusing progressively on the introduction of renewable energy systems to replace fossil fuels which can play a major role in reducing CO2 emissions [1]. Connected to these renewable alternatives is the intermittent character. Solar energy, as a pollution-free, inexhaustible, and affordable energy resource has vast potential [2]. However, one of the barriers for solar energy technology is rooted in the mismatch between energy supply and demand. Therefore, energy storage is proposed as a necessity to address this mismatch.
Thermochemical energy storage is a promising candidate for energy storage as it offers a high energy storage density and almost no heat loss. Thermochemical heat storage is based on reversible sorption reactions used to store energy. In this study we have looked at zeolite as a heat storage material due to its high stability [3]. However most research up to now on packed bed reactors for heat storage has primarily been based on models where the temperature is measured. In this study we have used a 1.5 T whole-body MRI scanner (Gyroscan, Philips) in order not only the measure the temperature but also the moisture as this is driving the heat storage reaction. In order to do so we have made use of a home-built insert which gives is the possibility to simultaneously measure both the moisture and temperature distribution in our packed-bed reactor. In this study we have made use of a glass reactor diameter of 60 mm and a length of 75 mm. The material used is the Zeolite 13X. Both the temperature of the air at the inlet and outlet are measured, whereas we can also control the RH of the inlet between 0-98% and the the temperature can be up controlled up to 220 oC so we can also study the recharging. The glass reactor is insulated with 20-30 mm of Rockwool.
From our measurement we see that the temperature front position is ahead of the moisture front position. Analyzing the moisture front velocities, assuming 1D instant adsorption, results in an accurate prediction of the front velocity with respect to the measured moisture front velocity. Comparing the temperature front velocity to moisture front velocity, it has been shown that the temperature front travels faster than the moisture front. That the temperature front leads the moisture front can be understood, since the temperature front velocity is dictated by the forced airflow velocity and the moisture front velocity is determined by the forced airflow velocity multiplied by a retardation factor caused by the sorption behavior of zeolite.
Analysing the moisture uptake showed that there is hydration ahead of the moisture front caused by a second hydration front. This has also been observed in the relative humidity at the outlet, multiple points of increase are observed, an increase in RH indicates that less water is being adsorbed, which is caused by a front breakthrough. This confirms that two fronts are present, a main front and a wall front due to wall channeling caused by a local higher porosity.

Participation:

In-Person

References:

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357

Numerical modeling of seismic monitoring of spatial saturation distribution in loosely deposited sands

Author: Tengfei Deng[1]

Co-authors: Olaf Hellwig [2]; Felix Hlousek [2]; Dominik Kern [1]; Stefan Buske [2]; Thomas Nagel [1]

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Extensive mine dumps consisting of loosely deposited sands have been created as a result of open-pit lignite mining, with a risk of soil liquefaction under high water saturation and a corresponding initiating event. In this context, the saturation spatial distribution and its change are critical factors in assessing the regional liquefaction potential. It is challenging to map the saturation distribution at large spatial scales owing to the complex properties of loosely deposited sands. In order to understand the spatial and temporal variations of saturation in loosely deposited sands, based on the sensitivity of P-wave velocity to saturation, seismic methods could be employed as a complement to other techniques. This method often uses empirical correlations established in the lab for the seismic inversion at the field-scale. However, wave propagation in porous media is frequency-dependent, especially between the ultrasonic frequency range and seismic frequency range. For the sake of building the bridge among the different frequency ranges, accurate wave propagation numerical modeling tools are required. To this end, a set of customizable codes, including poroelasticity and elasticity, is developed in the FEniCS library, which takes into account partial saturation and porosity dependence of stiffness, permeability, and other quantities. Moreover, the frequency-dependent poroelastic model and non-Biot damping are implemented by employing a memory variable. First, a series of synthetic cases are employed to benchmark the code by comparison to analytical solutions, and the applicability of different models is investigated by plane wave analysis. Then, the applicability of the different models is investigated on three different scales: ultrasonic lab-scale measurement, pilot plant site and field survey. Comparing numerical results and observed data, the poroelastic model provides better velocity prediction in the ultrasonic measurement scale and pilot plant survey scale. Nevertheless, the poroelastic and elastic codes have almost identical predictive capabilities at the field scale but can incorporate different information during parameterization/inversion. The different results obtained can provide a reliable basis for the migration of laboratory data to the field.

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Energy Transition Focused Abstracts:

MS03 / **358**

An REV-scale model for dissolution of porous rocks

Author: Anthony Ladd[1]

Co-authors: Liang Yu [1]; Piotr Szymczak [2]

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Modeling subsurface flow and reactant transport on large (km) scales necessarily involves statistical descriptions of the underlying pore space. Pore-scale models are one route to the constitutive models needed to close the macroscopic transport equations, but when the reaction rate is high, classical upscaling methods fail. Here we describe a different upscaling scheme based on concentration fluxes rather than concentration fields. The upscaling is based on two observations from finite-volume (OpenFOAM) simulations of dissolution in perioidic porous materials. First, that the concentration field in each unit cell of a periodic array can be mapped to a universal spatial distribution that depends only on the incoming concentration flux. Second, that the shape (and therefore the porosity) of a dissolving unit cell in one position can be mapped onto a different unit cell at a different time. These two observations can be combined into an ansatz for the time-dependent concentration field in a dissolving (initially periodic) array of grains. I will present numerical results in support of this ansatz over a range of Peclet and Damkohler numbers.

Based on the proposed ansatz, we have developed an REV-scale model for the dissolution of a porous matrix, which is valid for all Damkohler numbers. The predicted porosity evolution is compared with pore-scale simulations in the Figure, shows results for a square array of disks at Peclet numbers of 20 (left column) and 200 (right column); the rows have Damkohlet numbers of 0.02, 2, 200, and infinity. (transport limited kinetics). The symbols indicate the model predictions in different unit cells, and the solid lines are pore-scale simulations.

At low Damkohler numbers (Da < 1), the REV model can be approximated by a continuum theory. In both cases (REV and continuum) a single constitutive model is all that is required. It accounts for the fraction of the incoming flux to the unit cell that is absorbed by the solid. It can be determined by pore-scale simulations of small samples.

Recently, we have extended the REV model to include a spatially varying macroscopic flow. The key idea is that the concentration fluxes leaving a unit cell (or REV) are distributed in proportion to the fluid volume flux. This approximation is valid whenever the REV-scale Peclet number is greater than 1, or when the reactant within the unit cell is well mixed. The fluid velocity can be derived from the porosity-dependent permeability of the unit cell, which can be determined along with the effective mass-transfer coefficient from pore-scale simulations on small samples.

This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division under Award Number DE-SC0018676, and by the National Science Center (Poland) under research Grant No. 2012/07/E/ST3/01734.

Participation:

In-Person

References:

Yu, L., Szymczak, P., Ladd, A.J.C., 2022. Dissolution of periodic arrays of grains: Upscaling of pore-scale simulations with fast reactions. Chemical Geology 592, 120687

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Poster / 359

Reactive transport modeling in aqueous environments using the Nernst–Planck formulation

Authors: Po-Wei Huang[1]; Bernd Flemisch[2]; Chaozhong Qin[3]; Martin Saar[4]; Anozie Ebigbo[5]

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Water in natural environments consists of many ions, which exert electric forces on each other. We discuss whether the coulombic effects are relevant in describing mixing and reaction processes in natural environments or laboratory experiments. A typical model for electric interactions in dilute aqueous solutions is the Nernst–Planck equation.

Using FEniCS (fenicsproject.org) and Reaktoro (reaktoro.org), we solve the Nernst–Planck transport and equilibrium reactions of the ionic species in water. By comparing numerical simulations to reaction-driven flow experiments performed in a Hele-Shaw cell, we show that the electric interactions between ions can be relevant in mixing and reaction processes. We further discuss the numerical techniques in solving the Nernst–Planck system. In microfluidic experiments considering the mixing of aqueous fluids or electrokinetic effects, the Nernst–Planck equation can be essential to describe fluids' behavior.

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MS10 / 361

Dynamics of water films during wetting and drying cycles in porous media

Author: Gijs Wensink[1]

Co-authors: Maja Ruecker [2]; Veerle Cnudde [3]; Laurenz Schroer [4]

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[2] *Department of Mechanical Engineering, Eindhoven University of Techology*

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Wetting and drying cycles in porous media are encountered in many natural systems, as well as engineered systems. Soils are exposed to these cycles many times, as water infiltrates during rain and dries out afterwards. These cycles are also important in cyclic usage of underground reservoirs, for example for storage of natural gas or hydrogen [1]. Important during gas storage is to retain a high injection or extraction potential from the reservoir. This depends largely on the relative permeability of the liquid and gas phase.

While water largely fills the pores at high saturation, it mostly forms water films on the pore surface of water-wet rocks at lower saturations. These water films swell ahead of the main displacement front during imbibition, and can snap off to cause trapping of gas phase clusters in the pore space [2]. The films can also evaporate into dry gas and precipitate minerals that exceed the saturation limit onto the pore surface [3]. This can eventually lead to blocking of pore connections and decrease well injectivity [4]. In porous soils containing clays, wetting and drying cycles can lead to expansion or shrinkage of the medium itself, leading to a change in mechanical behavior of the soil [5].

In order to understand the likelihood of events such as snap-off or mineral precipitation in porous media, it is crucial to know how the water films are distributed on the rock surface during displacement processes. Since these water films can have a thickness of a few microns or less, many imaging techniques, such as micro-computed tomography or optical microscopy are able to capture those, but are limited in quantifying them. Atomic force microscopy (AFM) is able to detect fluid films on nanometer scale [6], and with this technique, we can track their configuration on the rough features of the internal pore surface.

We use AFM to investigate the dynamic behavior of water films in porous rocks during wetting and drying cycles. Using force measurements, we track the thickness of the fluid film on the surface over time and characterize the swelling or shrinkage rate at different locations. We relate the observed dynamics to sub-pore scale events such as triple phase contact point jumps and pore-scale displacement events, which are imaged by dynamic micro-CT (EMCT at Ghent university [7] through the EXCITE network*). This study will give fundamental insights into the role of water films on multiphase displacement processes at different length scales, and can be used for construction of more accurate and physics-based predictive models for multiphase flow in porous media.

Participation:

In-Person

References:

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Poster / 362

Water-Oil Relative Permeability determination in 2D micromodels of vugular porous media

Author: Jesús Daniel Fernández[1]

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It is estimated that 50% of world oil production comes from naturally fractured carbonate reservoirs. One of the biggest challenges in this type of formation is its heterogeneous nature. Besides the presence of fractures that longitudinally connect the porous media, vugs at different scales and distributions are scattered throughout the porous matrix. These cavities cause fluid flow characteristics to significantly differ from those of homogeneous reservoirs and bring the need to evaluate equivalent petrophysical properties of the system. Permeability is a key property to understand and predict operations involving one or more phases flowing through porous media. However, for vugular formations, obtaining representative rock samples to perform measurements is especially difficult. In addition, interpreting equivalent relative permeability maps can be challenging, since fluid saturation may not be uniform throughout the porous and vugular space.

Microfluidics approaches by means of artificial porous media micromodels have been widely used for pore-scale multiphase fluid flow visualizations, in order to relate macroscopic fluid flow properties to microscopic displacement mechanisms. When these devices are coupled with precise pressure drop measurements, additional information gathered from permeability determination could lead to important advances in this area. For example, improving the interpretation of data that are fed into simulations or that are obtained from core-flooding experiments.

In this study, a microfluidic approach is used to determine the water and oil relative permeability curves and phase distribution profiles in 2D micromodels of vugular porous media. It involved

prototyping a randomly-constricted porous matrix, incorporating different designs of vugs, and microfabrication of PDMS-glass micromodels. Steady-state water-oil injection experiments were performed in these devices at different fractional flow, monitoring the dynamics of the pressure drop and visualizing the fluid displacement at the pore scale. Live-image acquisition through fluorescence microscopy made it possible to examine the evolution of the saturation of water and oil phases. The direct comparison between the relative permeability curves of well-characterized vugular porous media and its porous matrix showed that the incorporation of vugs leads to (i) higher equivalent absolute permeability, especially with longer cavities and higher vug density, (ii) increased oil occupancy in the porous matrix, due to less efficient water invasion into the porous matrix, and (iii) higher relative permeability to water, which flows preferentially through the vugular space. These results are consistent with the oil-wet nature of micromodels, since the vugs are offering less capillary resistance to the flow of the non-wetting phase. Our low-cost microfluidic approach will likely allow us to systematically study more complex vugular-fractured systems.

Participation:

In-Person

References:

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Traveling wave solutions describing the foam flow in porous media for low surfactant concentration

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We present a foam displacement model with a separate balance equation for the surfactant concentration in the aqueous phase. We consider the gas mobility that depends on the surfactant concentration and the dynamic behavior of foam as Newtonian. We study traveling wave solutions for the proposed model considering a high initial water saturation (drainage scenario) and varying the injected water saturation. The traveling wave solutions are studied using phase portrait analysis

and validated with direct numerical simulations. For surfactant concentration at the injection and initial conditions above the Critical Micelle Concentration (CMC), we only found traveling wave solutions in the case when these concentrations are equal. For surfactant concentration at the injection and initial conditions below the CMC, we found traveling wave solutions whenever surfactant concentration at the injection is greater or equal to that at the initial condition.

Participation:

In-Person

References:

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MS13 / 364

Bicontinuous Microemulsion in Porous Matrices

Author: Margarethe Dahl[1]

Co-authors: René Haverkamp [2]; Larissa Doll [1]; Thomas Hellweg [2]; Stefan Wellert [1]

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Wicking is the spontaneous imbibition due to the negative capillary pressure created at the liquid-air interface 1. The wicking of simple fluids, such as water and organic solvents is well understood for a long time [2]. This well defined situation becomes more complicated in the case of complex fluids with an internal structure on the nanoscale. Then, competitive wetting and confinement effects play an important role and influence both, the behavior of the complex fluid inside the porous matrix and the inner structuring of the fluid. The latter can result in changes in phase behavior and other fundamental properties. To explore these effects we use bicontinuous microemulsions in the ternary phase system (water/octane/C\textsubscript{10}E\textsubscript{4}) as model complex fluid and controlled-pore glasses as confining matrices (CPG). Understanding the influence of geometrical restrictions yields both, fundamental insights and importance for applications, e.g. decontamination and enhanced oil recovery.

For a deeper understanding of these effects, of the spontaneous imbibition of a bicontinuous microemulsion and its components into the CPGs is investigated. In our study, we explore the wicking with the Washburn approach. In this approach the wicking of a test liquid is monitored gravimetrically, as shown on the right side in figure 1. Effects of the traversed matrices are studied by using various CPGs with pore diameters between 75 –1000 Å and porosities from 55% to 80 %. The naturally hydrophilic surfaces of the CPGs were hydrophobically modified to analyze the impact of the surface polarity. The bicontinuous microemulsion shows a more universal wicking behavior than the tested pure liquids.
Imaging techniques (cryo-SEM) and small angle scattering (SANS, SAXS) are used to investigate the microemulsion phase structure inside the porous matrices. In this talk, the results of these combined experiments will be presented and discussed.

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Participation:

In-Person

References:

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MS10 / **366**

3D observation of (nano)-cellulose fibers network by multiscale imaging techniques: from nanometer to millimeter scale.

Authors: NELLY PADILLA BELLO[None]; Christian Geindreau[1]; Sabine Rolland du Roscoat[1]

Co-authors: Mathilde Rota [2]; Hélène Curmi [2]

[1] *University Grenoble Alpes, Grenoble-INP, CNRS, Laboratoire Sols-Solides-Structures-Risques (3SR)*

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The end of single plastic packaging is scheduled in Europe around 2040.
Cellulosic materials such as paper and cardboard are today the only viable bio-sourced alternative, biodegradable and already recycled, which can reach a mass market. Paper is a multiporous material

with a large surface area accessible to contaminants. The transport of contaminants via the gas phase or cycles of (ad)sorption/desorption between the different components (shipping boxes, paper, and board), between the fibers and finally between the food particles (powder, grains, flake) is supposed to be the critical factor in food packaging. The roles of the connectivity of voids, micro-, and macropores, and the effects of the entanglement of fibers, specific surface area, surface composition, and relative humidity are poorly understood.

The aim of the present work is to characterize the 3D microstructure of a new type of paper for packaging. To reach the desired barrier properties, this new material combines a 200 micron thick paper with a 20 micron thick MFC film: (i) the paper is made of cellulose fibers with a diameter size range of a few micrometers and millimeters, (ii) the MFC film is made of a network of microfibrillated cellulosic fiber with sizes of about 20 to 50 nm in diameter and 500 to 1500 nm in length and ensures the barrier propeties. The MFC film is sticked on the paper or cardboard following a wet lamination technique 1.

In the past, several imaging acquisition techniques have been used to characterize the cellulose material such as paper and MFC film [2,3]. These techniques reveal relevant information about the microstructure but depend on the object desired to observe and the pixel size achieved by the source. Therefore, in our case, since the fiber size range is wide and depends on each layer, a single imaging technique will not reveal the microstructural information of the whole bilayer network. Thus, several techniques must be combined to accomplish the full 3D characterization of the bilayer network.

In the present work, the bilayer material has been imaged by either micro or nano synchrotron tomography, and using a FIB-SEM. The 3D X-ray images were performed in ID16B and ID19 beamlines at European Synchrotron Radiation Facility (ESRF). ID16B beamline was used to scan the MFC film at a pixel size of 25 nm/pixel and ID19 beamline was used to characterize the paper and interphase between paper and MFC layer at a pixel size of 0.36 μm/pixel. In parallel, the MFC layer was also scanned using a FIB-SEM technique to reach smaller pixel size (5 nm/pixel) and to highlight details of the MFC film. Despite some artifacts captured by the imaging techniques which hindered the segmentation task, we present for the first-time full 3D reconstruction of this new material. The microstructural properties (porosity profile, specific surface area⋯) have been then computed. The obtained results suggest that there is no visible pore connectivity in the MFC film which is consistent with the results of nitrogen adsorption/desorption.

Participation:

In-Person

References:

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Extraction of pore structure information in nanoporous media with sub-resolution porosity using X-ray nanotomography

Author: Xuanqing Lou[None]

Co-author: Zuleima Karpyn [1]

[1] *Penn State U.*

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The knowledge of pore network in a porous medium is critical for the accurate prediction of its structural properties and transport mechanisms. Non-destructive X-ray micro-/nano-tomography (micro-/nano-CT) enables the generation of three-dimensional (3D) CT images of a porous medium at micro and nano scales, thereby providing the opportunity to quantitatively describe the geometrical and topological characteristics of the 3D pore structure with a high-resolution. However, the nanosized pores in nanoporous media cannot be fully resolved due to the limited resolution. Consequently, the application of micro-/nano-CT imaging on nanoporous media with sub-resolution pores is underdeveloped. In particular, natural nanoporous media, such as unconventional rocks, often present more complex pore structures, posing great challenges for the description of their pore structure. In this study, a small section of natural Haynesville shale rock (1mm thick) was imaged by X-ray nano-CT with a resolution of 270nm, and the 3D digital image data was then visualized and analyzed by several image processing techniques to quantitatively extract pore structure information. A sensitivity analysis and segmentation technique were performed to obtain pore size distribution (PSD) in segmented pores with a high level of accuracy. On the other hand, a direct statistical analysis honoring a linear transformation between CT number and pore size was carried out on the sub-resolution volume. Results showed that the majority of the pores were below 270nm in equivalent diameter for this rock. The sub-resolution and segmented pores contributed 74% and 26%, respectively, to the total pore volume. The sub-resolution pores ranged in size from 10-270nm, while the segmented pore sizes ranged from 334nm to 10,114nm. Nitrogen adsorption and mercury intrusion porosimetry (MIP) were performed in order to validate the results obtained from nano-CT imaging. Although a discrepancy can be found when comparing different PSD curves, nano-CT imaging PSD with rational peaks falls in a reasonable range. The inconsistency comes from the assumptions of the different techniques. The calculated specific surface area (2.77×10^7 m^(-1)) was found to be reasonable compared to the values from nitrogen adsorption (3.02×10^7 m^(-1)) and MIP measurements (3.17×10^7 m^(-1)). These results indicate the practical feasibility of extracting the nano-scale spatial pore structure information in a nanoporous material from a single sub-resolution image. This study offers a workable solution to extract a representative volume of 3D pore space compared to other available image-based techniques. This will therefore lay a foundation for pore network extraction in pore-scale modeling, which will be applicable to different types of nanoporous materials.

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MS06-B / 368

Multiphase relaxation processes at the µm-to-cm scale during storage of gases in rocks

Author: Sharon Ellman[1]

Co-authors: Catherine Spurin [2]; Samuel Jackson [3]; Catrin Harris [4]; Ben Callow ; Shan Wang ; Gulce Kalyoncu ; Tom Bultreys [1]

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The interaction of gases and liquids in the subsurface has become highly relevant as subsurface carbon dioxide sequestration and hydrogen storage have been identified as key technologies to abate climate change. Gas mobility is affected by capillary trapping1, dissolution[2] and Ostwald ripening[3], as well as the capillary relaxation of the fluid/gas system, with important consequences for gas storage applications.

These processes can occur simultaneously within natural porous media and each have their own characteristic time and length scales. The time and length scales over which fluids relax to capillary equilibrium within geological porous media are poorly understood[4], particularly in the presence of small-scale capillary heterogeneity[5]. It is hence unproven whether a sufficient separation of scales exists between capillary relaxation and trapping, gas dissolution and Ostwald ripening to model these processes independently.

In this work, we investigated the coupled relaxation processes at the pore scale in a 25 x 45 mm Bentheimer sandstone sample, using the HECTOR micro-CT scanner at UGCT[6] to image the pore space at 10 µm resolution. Using a sample that was one order of magnitude larger than typically used in pore-scale investigations made it possible to study the effect of length scales where viscous forces and capillary heterogeneity come into play. We conducted core floods with post-drainage and post-imbibition relaxation, using nitrogen (as model carbon dioxide/hydrogen) and KI brine at a pore pressure of 50 bar. After each fluid invasion, the sample was isolated and maintained at a constant pressure. Preliminary results reveal significant differences between the relaxation processes after drainage and imbibition. Following drainage, the system appears to reach equilibrium almost instantly, with no visible changes in the fluid distribution being observed over the course of several hours. This is in stark contrast with the observations made during imbibition, where the system continues to change even 18 hours after imbibition is stopped.

Understanding relaxation, and all the processes associated with it, has implications for storage security and efficiency during carbon dioxide sequestration and subsurface energy storage.

Participation:

In-Person

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MS05 / **371**

Engineered soil-mycelia systems for slope stabilisation

Authors: Grainne El Mountassir[1]; Alireza Fathollahi[1]; Qi Zhang[1]

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Landslides in granular soils are often triggered by rainfall; this phenomenon and the underlying mechanism of water infiltration resulting in increased pore water pressured (reduced soil suction) and hence lower shear strength has been well documented for natural hillslopes worldwide. Globally, up to 350 fatal landslides are triggered by rainfall each year and individual events can cause thousands of fatalities (Kirschbaum et al., 2012). In Europe, up to 3.6 million people live in landslide prone areas with 8,000 to 20,000 km of roads and railways at risk of landslides, and associated annual economic losses of ~4.7 billion Euros (Haque et al., 2016). In many regions predicted changes in climate are likely to further impact the stability of slopes, driving the need for novel approaches for their management and maintenance. This research investigates the potential of engineered soil-mycelia systems to improve slope stability.

Filamentous fungi grow in the form of hyphae, tubular structures with diameters between 2-7μm. Hyphae branch out and fuse together forming a complex network, called the mycelium. Mycelia have attractive characteristics for use in ground engineering: evidence from natural analogues indicates that they can form massive, durable mycelia with individual organisms of Armillaria sp. up to 10 km2 in size and >1,900 years old found on forest floors in N. America (Ferguson et al., 2003). Furthermore, mycelia networks are resilient; dynamically responding to the environment and damage or disruption (Fricker et al., 2008). Different fungal species have varying growth requirements and forgagng behaviour which give rise to different mycelia architecture (e.g. dense diffuse mycelia, cords, rhizomorphs).

This study investigates the ability of saprotrophic basidiomycota fungal species to contribute to slope stabilisation. In order to identify suitable fungal species a screening study was conducted which investigated the ability of a number of different UK native basidiomycota species to (i) grow in non-sterile soils, (ii) induce water repellency and (iii) bind soil particles together. These were assessed via time-lapse photography and image analysis, water droplet penetration tests and via soil aggregate

stability tests. Results show that growth behaviour and resulting mycelium architecture influences the ability of fungi to bind soil particles. Basidiomycota fungi show promise for enhancing slope stability by reducing water infiltration during rainfall events, enhancing soil cohesion and improving soil resistance to erosion.

Participation:

In-Person

References:

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Advanced characterization of novel multilayer cellulose based material for food packaging

Authors: NELLY PADILLA BELLO[None]; Mathilde Rota[1]; Hélène Curmi[1]; Christian Geindreau[2]; Sabine Rolland du Roscoat[2]

[1] *The technical center of paper (CTP)*

[2] *University Grenoble Alpes, Grenoble-INP, CNRS, Laboratoire Sols-Solides-Structures-Risques (3SR)*

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The demand for biobased, biodegradable, recyclable, and recycled material is a growing market. The consumers and policies in European countries encourage the circular economy and the replacement of single-use plastic packaging. Cellulose fibrous materials, as a unique source recyclable and biodegradable, offer an alternative economical and technological solution to the problems caused by plastics. However, these materials are multiporous material with a large surface area accessible to contaminants.

An alternative to limit the migration of contaminant through these cellulosic materials is to add a functional barrier to the packaging, such as an MFC film. A MFC film is a thin (typically 20 micron thick) and dense fibrous network entirely made of microfibrillated cellulose (MFC), whose fiber sizes range from micrometers to nanometers. These films are biodegradable and recyclable, and can be employed to coat paper and paperboard by using a technique called wet lamination 1. The wet lamination combines filtration, pressing, and drying process to produce a multi-scale structures, i.e. bilayer materials. These materials have promising barrier properties for food packaging [2,3], but the role of the microstructure on the contaminant transport is poorly understood.

The project aims to understand the influence of the micro-structural features (the connectivity of voids, nano-, micro-, and macro-pores) of such bilayer material on their barrier properties. For that purpose, a MCF film of 25 g/m^2, produced from two sources of MFC has been produced and used to laminate three base materials: (i) a Gerstar HDS paper (80 g/m^2), (ii) a blotting paper (90 g/m^2), and (iii) a Cupforma Natura cardboard (195 g/m^2).

In the present work, we evaluate the barrier properties of the handsheet samples such as the absorption index, water vapor, and oxygen transmission rate. The obtained results are compared to standard results on the same material without any MFC film and are analysed in the light of microstructural observations performed by various imaging techniques. The findings suggested that the MFC film may cover the pores of paper which hinder the absorption of grease molecules, and the transport of water vapor and oxygen molecules through the fibrous network. The use of MFC as surface coating on various base papers considerably improve their barrier properties. However, the performance of the membrane will depend on the basic weight of the MFC film and the fiber size of the MFC film.

Participation:

In-Person

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Poster / 373

Numerical analysis of axial compression impact on the hydrodynamics of open-cell foams

Author: Alaa-eddine Ennazii[None]

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eX-Poro-HydroDynamique lubrication (or XPHD lubrication) presents a different scientific approach to dealing with tribological problems. It's an innovative inter- and multidisciplinary research topic which offers a promising sliding solution for various applications, such as bearings, thrust bearings, various guide components, etc. Its applications in both biological systems, and industrial systems : soft porous squeeze damping or soft porous lubrication are very broad and important. XPHD lubrication is a lubrication mechanism of biomimetic inspiration which features an additional parameter to the system "the porous media". It consists of self-sustained fluid films generated within compressible porous layers (CPL) imbibed with liquids in replacement for using the fluid film only as in the classic lubrication system. Soft and porous structures imbibed with liquids generate a high load support under compression, the load support is generated through the resistance to flow inside the porous material. During compression, the resistance to flow and load support increase, the greater the compression level, the lower the porosity and corresponding permeability. The main objective of this work is to understand the behavior of the fluid flow inside the porous structures when subjected to axial compression stress. In the scientific literature, the works studying the flow in compressible materials are essentially experimental because of their very complex geometrical shape 1, [2], [3], the CFD (Computational Fluid Dynamics) simulations offer an economical solution to study the performance of this new concept of lubrication. To create the geometry, the morphological structure of foam samples is reconstructed at different levels of compression rates from 3D X-ray microtomography. This is achieved by using a commercial software (Avizo) that allows to process 3D images and create FE/CFD models suitable for numerical analysis [4]. The numerical simulations of flows will be performed with the solvers icoFoam and simpleFoam of the OpenFOAM [5] framework for steady-state incompressible laminar and turbulent flows, making it possible to study different fluids and porous materials. The performed simulations were made with an open-pore polyurethane foam with 96% porosity using five compression rates for creating the different geometries. For the fluid we used water and a hydraulic oil ISO VG 46 to see the impact of the viscosity on the flow. The analysis of the simulations shows the impact of the solid compression on different parameters, such as the decrease in permeability as function of the compression rate, the anisotropy of the flow within the compressible structure and the actual increase in the tortuosity generated by the compression of the solid and the variation of the porosity.

Participation:

In-Person

References:

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MS21 / **374**

A linearised closure approach for averaged inertial and compressible flows

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An important challenge in up-scaling inertial and compressible flows is the treatment of the non-linear terms remaining in the closure problems 1. As a consequence of these non-linearities, current approaches require to solve closure problems that are themselves dependent on the local averaged flow [2], thus limiting the benefits of the upscaling procedure.
Here, a methodology is proposed wherein the non-linear closure problems are linearized according to relevant dimensionless numbers using power series. Indeed, dimensional analysis of the closure problems arising in the volume averaging procedure of inertial and slightly compressible flows indicates that non-linear terms are controlled by dimensionless parameters such as the Reynolds number and the dimensionless compressibility coefficient [3]. For each order of the power series decomposition, linear and intrinsic closure problems are determined. Finally, the effective properties of the medium for small values of the dimensionless numbers are obtained by truncating the developments to the appropriate order. One of the main advantages of the proposed method is that it does not require to solve the full closure problems for each value of the local averaged flow.
After assessing the validity of this approach against numerical solution of the corresponding non-linear closure problems, the global permeability tensor, including contributions from inertia (Forchheimer term) and compressibility, is determined. Finally, generalization of this methodology to other types of non-linear flows such as flows with temperature-dependent properties is examined.

Participation:

In-Person

References:

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MS03 / **375**

Exploring the limits of semi-analytical matrix diffusion

Authors: Matthew Sweeney[1]; Jeffrey Hyman[1]; Konstantin Lipnikov[1]; Aidan Stansberry[1]; John David Moulton[1]; Hari Viswanathan[1]; Philip Stauffer[1]

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Matrix diffusion is a critical process to capture in many subsurface applications in low permeability fractured rocks. In most discrete fracture network (DFN) models, a semi-analytical description of matrix diffusion is adopted in conjunction with Lagrangian particle tracking methods. However, the solutions to semi-analytical matrix diffusion are based on simple fracture networks, i.e., single fractures or multiple parallel fractures where fracture spacing is well-defined. Natural fracture networks can have spatially variable fracture spacing, orientations, and lengths, which could impact the accuracy of semi-analytical matrix diffusion, but has not been quantified to date. In this work we leverage new developments in the dfnWorks software suite to generate discrete fracture matrix (DFM) models to compare solute breakthrough in DFNs with semi-analytical matrix diffusion and DFMs with an explicit description of matrix diffusion. We are able to generate high resolution DFM meshes using a 3D Poisson disc sampling algorithm, where the faces of the fracture mesh conform to the faces of the matrix mesh. Governing equations for flow and transport in the coupled system are solved using the Amanzi Multiphysics code. We first verify the implementation of the explicit matrix diffusion in Amanzi for a single fracture against the semi-analytical solution. Then we systematically increase the complexity of the underlying networks to determine how well the semi-analytical matrix diffusion compares with the explicitly captured matrix diffusion and link the accuracy back to quantifiable fracture network properties.

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MS15 / **376**

Physics-Informed Deep Learning for Reactive Transport of Volatiles in Cellulose-based Porous Media

Authors: Alexandra Serebrennikova[1]; Raimund Teubler[2]; Ekaterina Baikova[3]; Eduardo Machado Charry[4]; Karin Zojer[4]

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Simulating the transport of gasses or liquids through porous media is challenging when the complex geometry of real systems is to be considered, especially when transport is accompanied by sorption and/or chemical reactions. This complexity challenges traditional numerical solvers in their ability to capture the intricate details of the system in an accurate yet feasible manner.

This contribution focuses on creating a mesh-free modeling framework for studying the reactive transport of volatile organic compounds through the complex micro-structure of papers. Previous studies 1 show that due to the chemical and physical interactions the organic volatiles exhibit sorptive behavior during their migration through the cellulose-based porous medium. This behavior is influenced by a combination of material properties, including the polarity of the organic compound, its diffusivity in the porous and solid phases of the paper, and the paper's micro-structural features such as porosity and tortuosity.

The underlying physics of the process is described by a system of non-linear partial differential equations (PDEs). The PDEs account for the diffusion of organic volatiles through the paper material as well as the adsorption and desorption of the compounds on the paper's surface. Due to the non-linearity of the PDEs and absence of analytical solutions in most of the cases, the inverse problem of determining the material properties based on experimental data is difficult to solve using regression models. In our previous work [2], we demonstrated on an example of dimethyl-sulfoxide (DMSO) migration through paper, how physics-informed neural networks (PINNs) can be successfully applied to solve inverse and forward problems in the case of one-dimensional transitive transport through paper.

Based on experimental migration data for DMSO and n-C14H30, current work extends this approach to two- and three-dimensional systems by incorporating micro-structural information obtained via micro-CT measurements of paper into the framework of PINNs domain. In this fashion the geometrical features of paper material are implicitly included in the formulation of the governing PDEs. We further decompose the domain of the solution functions into two parts: one representing the porous phase of the paper micro-structure, and the other representing the solid phase. We use separate PINNs to search for the solutions in each phase, merging them together at the interface by applying boundary constraints that govern the sorption process. On the one hand, this approach allows for a more accurate representation of the physical system based on the real geometrical data. On the other hand, using multiple PINNs is beneficial for the systems with complex topology where the solution functions show discontinuities on sharp interfaces and therefore require more flexible approximation functions.

Participation:

In-Person

References:

1 Hoffellner, Lisa and Henoegl, Elias M. and Petschacher, Patrick and Schennach, Robert and Leitner, Erich, (2021), The Interaction of Cellulose Thin Films With Small Organic Molecules—Comparability of Two Inherently Different Methods., Frontiers in Chemistry, vol. 9. https://doi.org/10.3389/fchem.2021.769022

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Poster / 377

Development of a micromodel design algorithm for heterogeneous reservoir rocks

Author: Sebastian Hogeweg[1]

Co-authors: Calvin Lumban Gaol [1]; Birger Hagemann [1]; Leonhard Ganzer [1]

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The utilization of microchips to study fluid flow processes in porous media has gained high popularity in recent years. The silicon structures between two glass plates allow the visual observation of various processes (e.g., EOR and microbiology during underground hydrogen storage) and assess their suitability for large-scale applications. Nowadays, a wide field of designs ranging from artificial structures to structures based on µ-CT images is available. The representation of pore space geometry for a specific rock is critical, which led to good workflows for designing pore structures from µ-CT images in the past. However, many displacement mechanisms are also influenced by heterogeneities of rock core samples on the macro scale. Applying existing micromodel design algorithms on strongly heterogeneous rocks often leads to a poor outcome. Relatively large areas with inaccessible or dead pores could be created, making experimental execution more difficult. This study extends an existing procedure by adding certain steps to improve the representation of pore geometry on the microchip. Using the Efros Freeman image stitching algorithm, the mask based on µ-CT images is homogenized to make optimal use of the area of the microchip. A gradient map is created based on the petrophysical parameters, which locally transforms the homogeneous mask into high and low permeable/porous zones. The low permeable domains compose circular shapes with a transition zone into the high permeable region. The petrophysical properties of the chip were fitted using pore-scale simulation in an iterative process to the rock sample.
In general, this algorithm is useful for the development of heterogeneous structures for micromodels. The resulting design combines a high level of pore space representation with the suitability for execution of complex flow experiments with a focus on visual investigations in porous media.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS12 / 378

The role of pore fluids in supershear earthquake ruptures

Authors: Pedro Pampillon[1]; David Santillan[2]; Juan Carlos Mosquera[1]; Luis Cueto-Felgueroso[2]

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The intensity and damage potential of earthquakes are linked to the speed at which rupture propagates along sliding crustal faults. Most earthquakes are sub-Rayleigh, with ruptures that are slower than the surface Rayleigh waves. In supershear earthquakes, rupture is faster than the shear waves, leading to sharp pressure concentrations and larger intensities compared with the more common sub-Rayleigh ones. Despite significant theoretical and experimental advances over the past two decades, the geological and geomechanical controls on rupture speed transitions remain poorly understood. Here we propose that pore fluids play an important role in explaining earthquake rupture speed: the pore pressure may increase sharply at the compressional front during rupture propagation, promoting shear failure ahead of the rupture front and accelerating its propagation into the supershear range. We characterize the transition from sub-Rayleigh to supershear rupture in fluid-saturated rock, and show that the proposed poroelastic weakening mechanism may be a controlling factor for intersonic earthquake ruptures.

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MS20 / **379**

In Vitro Characterization of Lingering Red Blood Cells In Capillary Networks

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[2] *Department of Mechanics, Mathematics and Management, Polytechnic University of Bari, 70125, Bari, Italy*

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Introduction:
The distribution of red blood cells (RBCs) in the microvasculature is an important factor for the supply of the tissue with oxygen. It is known that the RBC distribution is spatially and temporally heterogeneous. One of the causes for the heterogenous distribution are lingering RBCs (LRBCs), i.e., RBCs which remain temporarily stuck at the apex of diverging bifurcations[1–3]. However, the lingering of RBCs has not yet been fully characterized. Therefore, we investigated the behaviour and properties of LRBC in an in vitro model of a microvascular bifurcation.
Methods:
A PDMS microfluidic device featuring a symmetric bifurcation of microchannels mimicking the dimensions of capillaries (channel width 9.6 um) was perfused with rabbit RBCs suspended in a plasma-like solution ($\bar{u}_{RBC} \approx$ 0.68mm/s, Hematocrit = 10 %)[4]. An image sequence (Eclipse Ti-e, Nikon) of 4000 video frames of RBCs flowing through the bifurcation was recorded using a high-speed camera

(395 frame/s, ORCA-Flash 4.0, Hamamatsu). The frames were pre-processed with a custom-written script[4], and every RBC was then tracked by particle tracking velocimetry[5] to determine position and velocity.
The transition time constant (τ) was used to discriminate between a LRBC and a non-lingering RBC (NLRBC) where τ is the time spent by the RBC in the bifurcation region divided by the mean time of all RBCs in this region. An RBC is considered lingering if it spends 50% more time in the bifurcation region than normal (LRBC τ>1.5 and NLRBCs τ<1.5).
Results:
In total, 378 bifurcation events were tracked. Out of these, 53 (14%) were classified as LRBC. Inspection of the lateral position of LRBC and NLRBC, indicated that LRBCs were flowing in the center of the parent vessel (PV, upstream of the bifurcation region), whereas the lateral position of NLRBCs was bimodally distributed with the two modes one eight of the channel width away from the centerline. Quantitative analysis confirmed that 96.2% of LRBCs were within one eighth from the centerline, whereas only 52.3% of the NLRBCs were in this region. After the bifurcation region, i.e. in the daughter vessels (DV), LRBCs were positioned closer to the inner wall (98.1% on the inner half width of the channel). In contrast, NLRBCs were more centered (28.9% on the inner half width). The mean RBC velocity in the DV was $\bar{u}_{NLRBC}$ = 0.31mm/s for the NLRBC and $\bar{u}_{LRBC}$ = 0.21mm/s for LRBCs. In the PV the difference between the LRBC and NLRBC was lower ($\bar{u}_{LRBC}$ = 0.70mm/s, $\bar{u}_{NLRBC}$ = 0.67mm/s).
Discussion:
In the PV, the only significant difference between LRBCs and NLRBCs was the lateral position. In the DV, the LRBCs were slower and stayed near the walls (as opposed to NLRBCs which were faster and more central). This different behaviour of LRBCs and NLRBCs is expected to result in a bifurcation bias in the next diverging bifurcation, which has been described previously as the history effect[3,4]. Our results support the presence of the history effect and indicate LRBC should be taken into consideration when studying RBC distribution in capillary networks.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS16 / 380

A Knowledge-Driven Reduced-Order Model with a data-driven corrector for thin porous media

Authors: Alaa Armiti-Juber[1]; Tim Ricken[1]

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Thin, porous media are ubiquitous in several environmental, industrial and engineering fields. Examples of such media are soil, aquifers, filters, fuel cells, in addition to some biological tissues such as cartilage. The dynamical behavior of such media is typically described and predicted using mathematical models in the form of coupled, nonlinear, partial differential equations (PDEs). Discretization of these PDEs leads to high-fidelity models requiring advanced numerical methods to provide simulations of high accuracy. Despite the huge advances in computational algorithms and computer chips, simulations might still be time-consuming. This can be problematic for many applications, such as design optimization, model-based predictive control, or clinical-time constraints.

For thin, porous media, the property of scale separation is naturally satisfied such that fluid's pressure is almost hydro-static in the small-scale direction. This property has been utilized to construct knowledge-driven reduced-order models using methodologies such as vertical averaging 1, asymptotic analysis [2,3], or rigid convergence analysis [4]. The resulting reduced model is typically a set of 1D equations describing the leading dynamics, mainly, in the large-scale direction. It has reduced computational complexity and provides proper approximations of the high-fidelity solutions. However, thin porous materials might violate the assumption of hydro-static pressure, e.g., due to high permeability gradients in the small-scale direction. For such cases, correctors must be considered to recapture the less effective dynamics. In [3], a knowledge-driven corrector is derived via asymptotic analysis for the higher-order terms in the asymptotic expansions. This corrector slightly improves the accuracy as it partially depends on the hydro-static assumption. Thus, we propose a novel data-driven corrector using projection-based methods, such as the method of proper orthogonal decomposition. For this, we use a training data-set of the errors induced by the reduced model at those configurations violating the assumption of hydro-static pressure. Numerical examples to validate the method are also performed.

Participation:

In-Person

References:

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Experimental study on microscopic mechanism of shale oil development by supercritical CO2/H2O huff -n- puff

Authors: Xiaomei Zhou[1]; Lei Li[None]

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Shale reservoirs have very poor porosity and permeability, rich in organic matter and clay minerals, the primary recovery of horizontal well after volume fracturing is low, and the development effect of conventional stimulation method is poor, supercritical CO2/H2O mixed fluid huff -n- puff is a promising technology. As the most extensive gas displacement agent, supercritical fluid CO2 has the potential to efficiently develop shale oil. Compared with CH4 and N2, CO2 is more easily miscible with crude oil and increases the flow capacity of oil. Supercritical H2O is a better performing fluid than supercritical CO2, with higher solubility, wider diffusion and better reactivity, which can improve the coefficient of sweep and the efficiency of oil washing during displacement. This work aims to establish a microfluidic device to investigate the micro-mechanism of shale oil exploitation by supercritical CO2 huff -n- puff and supercritical CO2/H2O mixed huff -n- puff. According to the statistics of typical pore throat data of shale, a nano-scale micro etched glass model is established. Then, based on the microfluidic, the huff -n- puff process in porous media was analyzed from the aspects of seepage characteristics, microscopic mechanism and residual oil distribution. The results show that the micro-mechanism of shale oil production by supercritical CO2 huff -n- puff is mainly the miscible phase mechanism of dissolution and extraction, the carrying extraction and compression expansion mechanism. The presence of water has a certain adverse effect on the mixing of oil and gas. Considering the oil-pore-throat contact relationship, the remaining oil can be divided into five flow forms: cluster, porous, angular, columnar and film. With the increase of gas injection pressure, the production trend of different types of remaining oil is different, and the degree of discontinuous phase of remaining oil is increasing. This work will be of great interest to operators looking for new ways to improve recovery from shale reservoirs.

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Energy Transition Focused Abstracts:

MS03 / **382**

Impact of artificial topological changes on flow and transport through fractured media due to mesh resolution

Author: Aleksandra Pachalieva[1]

Co-authors: Matthew Sweeney [2]; Jeffrey Hyman [1]; Emily Stein [3]; Rosie Leone [3]; Hari Viswanathan [1]

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We performed a set of numerical simulations to characterize the influence of mesh refinement and upscaling on flow and transport properties in fractured porous media. We generated a set of generic three-dimensional discrete fracture networks at various densities, where the radii of the fractures were sampled from a truncated power-law distribution, whose parameters were loosely based on field site characterizations. We also considered five network densities, defined using a dimensionless version of density based on percolation theory. Once the networks were generated, we upscaled them into a single continuum model using the upscaled discrete fracture matrix model presented by Sweeney, Gable, Karra, Stauffer, Pawar, and Hyman (2020). We considered steady, isothermal pressure-driven flow through each domain and simulated passive/conservative, decaying, and adsorbing tracers using a pulse injection into the domain. We calculated the effective permeability and solute breakthrough curves for each simulation as quantities of interest to compare between network realizations. We found that selecting a mesh resolution such that the global topology of the upscaled mesh matches the fracture network is essential. If the upscaled mesh has a connected pathway of fracture (higher permeability) cells, but the fracture network does not, then the estimates for effective permeability and solute breakthrough will be incorrect. Local false connections between fractures due to a coarse mesh result in more solute dispersion in the transport behavior, but to a smaller degree than if there is a mismatch in global connectivity. False connections cannot be eliminated entirely, but they can be managed by choosing the appropriate mesh resolution and refinement for a given network. Adopting octree meshing to obtain sufficient levels of refinement leads to fewer computational cells (up to a 90% reduction in overall cell count) when compared to using a uniform resolution grid and can result in a more accurate continuum representation of the true fracture network.

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MS20 / 383

Numerical methods for simulating flows in biological networks

Author: Tobias Koeppl[1]

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Network structures can be detected in almost every biological system, since they are often responsible for the transport of fluids, nutrients or oxygen. Such a network structure is for example a blood vessel network supplying organs with oxygenated blood or removing metabolic waste from the tissue 1. A further example is the root network of a plant, ensuring the water supply of the plant.

One way to obtain a realistic model for such processes is based on a decomposition approach. Thereby, the network structure is separated from the surrounding medium and different models are assigned

to both domains. Quite often the surrounding medium (e.g. tissue or soil) can be considered as a three-dimensional (3D) porous medium. In order to decrease computational costs while maintaining a certain degree of accuracy, flow and transport processes within the networks are modeled by one-dimensional (1D) PDE-systems. A coupling of the network and the porous medium model is achieved by first averaging the 3D quantities and projecting them onto the 1D network structure. As a next step, the difference of the averaged 3D and 1D quantities is computed and incorporated into the source terms of both the network and the porous medium model, where the source term of the 3D problem exhibits a Dirac measure concentrated on the 1D network [2].

In this talk, numerical solution algorithms for PDE systems arising in the context of this model concept, are presented. In particular, the performance of a finite difference method with a regularized Dirac source term is investigated [3,4]. Therefore, elliptic model problems with Dirac source terms and averaging operators are considered. Theoretical results are confirmed by numerical tests.

Participation:

In-Person

References:

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MS15 / **384**

Multiscale Rock Image Pore Structure Feature Identification, Quantification and Modelling using AI

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Due to the complexity of rock structure with features on scales ranging ten orders of magnitude, the multiscale fractured carbonates require more complex analysis tools than the macroscopic simulation approaches currently used which have been developed for and validated against siliciclastic rocks primarily. Digital Rock Technology (DRT) offers a means to determine the system's transport properties on a pore-scale basis. DRT allows the investigation of fluid flow mechanisms in a comprehensive setting (e.g. single/multiphase flow, reactive flow). Furthermore, pore network models (PNM) have been used to model complex rocks due to their superior efficiency (improved computational speed, carbon footprint, and scalability) and ease of characterising the porous media using representative geometrical and topological statistics. However, current PNM open-source codes rely on strict definitions of the pore elements with symmetrical convex bodies and pores which can be challenging or even impossible to define the necessary irregular pore geometries in carbonate. Moreover, PNM does not consider heterogeneous multiscale features like fractures and vugs, which are difficult to discriminate and segment but have distinctive flow properties that can critically change the overall system behaviour.

In this talk, we will present a novel machine-learning algorithm for the semantic segmentation of rock matrix, porous/vugular elements, fractures, and secondary mineralogy, which was optimised considering its accuracy, complexity (measured using the total number of parameters, number of operations, run-time, energy consumption, and carbon footprint), and explainability based on the Green-AI philosophy. After comparing several techniques, shallow machine learning methods were preferred due to their superior computational efficiency and explainability whilst achieving comparable segmentation accuracy. The workflow proposed is a hybrid algorithm relying on both region-based and filter-based techniques to achieve the best accuracy and speed. Firstly a 2.5D (slice-by-slice) analysis is performed to separate pores from larger features, with the size threshold selected via a Gaussian mixture model. Subsequently, the micro-fractures and pores are separated via watershed, and the resulting elements are separated into pore elements and over-segmented fracture elements. Following this procedure, pixel-level segmentation is performed to distinguish and potentially separate large fractures and vugs, using this more computationally intense method only on the uncertain areas, hence optimising performance. The matrix class is also analysed to identify secondary mineralogy, which has the potential to alter wettability.

Each feature class is further segmented into instances and idealised, creating a multiscale network. The pre-existing open-source codebase is expanded by increasing its flexibility to complex geometries and introducing multiscale features, which will remove one of the main weaknesses in current approaches. Moreover, fracture elements are also modelled distinct from pores, observing the typical flow regime. Validation of the algorithm against the solution via direct simulation methods (namely the finite volume method) and experimental results of known samples is ongoing.

The outcome of this research is that of a resource-efficient and explainable algorithm that can discriminate between pores, fractures and vugs (and optionally secondary mineralogy) enabling automatic linking of the semantic segmentation result with the pore-fracture-vug network extraction, hence improving the modelling accuracy.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / 385

Management of salt precipitation for large-scale CO2 storage projects

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CO_2 storage at climate-relevant scales will involve rapid deployment of projects worldwide in diverse geological settings, with each involving several millions of tons injection per annum. CO_2 transport also can be varied, with pipeline transport being supplemented by direct injection from ship or other land-based transport. Successful projects should have low risk of injectivity loss to be cost-effective for commercial implementation. Salt precipitation has been identified as a mechanism for injectivity reduction in the near wellbore region, especially for saline aquifer storage. Salt crystals can accumulate in pore throats as injected CO_2 evaporates residual water, which reduces permeability and blocks flow. Although salt precipitation can be treated effectively, poor management can lead to unwanted well shut-in and additional costs to industrial projects.

Salt precipitation has been documented to some extent in the field and has been extensively studied in experimental and numerical studies. Industry-standard simulation tools, both commercial and open-source codes, have the capabilities to model permeability reduction due to salt precipitation. Although the phenomenon does not appear to be a showstopper, one main challenge is to understand under what circumstances salt precipitation will require potentially costly intervention. First, CO_2 storage projects in saline aquifers to date have injected relatively small volumes of CO_2 and therefore negligible salt precipitation. Secondly, little is known about the impact of hysteresis under cycling CO_2 injection (e.g. direct injection from ships) that could enhance the risk of salt precipitation. Another challenge is understanding the correct laboratory protocols for experimental studies, which has been shown to have a significant impact on conclusions related to permeability reduction. Finally, it is often not clear how to translate lab observations in simple idealized systems to predictions at the field scale where geology, wellbore construction and multiphase flow behavior is significantly more complex.

In this study we perform a comprehensive review and analysis of knowledge, data and simulation capabilities related to salt precipitation and the realistic impacts for CO_2 storage injectivity. Using benchmarked simulation tools, we extend current analysis from small, pilot-scale injection in idealized settings to large-scale commercial deployment, particularly under cyclical injection conditions and heterogeneous flow conditions. We propose directions for future experimental and simulation studies to close remaining knowledge gaps. We also suggest guidelines for assessing and managing salt precipitation for large-scale CO_2 storage in realistic settings.

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Poster / 386

Multiscale Integration of Discrete Fracture Network and Pore Network Modes Focused on the Pore-Fracture Interface

Authors: Ciprian Panaitescu[None]; Kejian Wu[1]; Yukie Tanino[2]; ANDREW STARKEY[3]

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The characterisation and quantification of fractures are essential for the analysis of naturally or artificially fractured porous media. Moreover, fractures and faults can dominate flow across scales, from the reservoir to the core scale. Fractures often dominate flow at a larger scale, whilst, at the micro-scale, pore and micropore physics are highly important, and the fractures can act as a cross-scale link. The current study uses micro-CT images as the input for the flow analysis of fractured geological media, emphasising naturally fractured carbonates.

The method selected for this analysis is pore network modelling (PNM). This simulation approach idealises the porous medium as a network of elements (traditionally only focused on pores) connected by throats, significantly improving the cross-scale analysis capability and computational efficiency. Additionally, fractures have been modelled via discrete fracture networks (DFN) that can integrate multiple resolution scales. However, it is only recently that research has begun on integrating fracture and pore networks of data extracted from micro-CT scans, with fractures modelled with their characteristic flow physics (for instance, modelling the intra-fracture flow as a Couette rather than Poiseulle problem, as is typical for pore throats).

The current work integrates the discrete fracture network (DFN) and pore network, maintaining the size characteristic of each fracture element from DFN, hence maintaining improved interpretability, robustness and efficiency. The known issue of the intra-fracture impedance is solved by introducing a novel empirical relationship that accounts for the relative differences between the connection and position of every fracture-adjacent throat. Artificial neural networks and stochastically fitted parameterization solutions are considered and compared. The data for training, validation and testing is obtained by analyzing varied real and semi-synthetic micro-CT cases, using the direct simulation (via the finite element method algorithm implemented in the OpenFOAM code) and using the results as ground truth.

This analysis result improves the prediction accuracy and efficiency of network models when tackling fractured porous media and cross-scale analysis, particularly improving the flow boundaries between fractures and pores and harmonising with previous research concerning pore-to-pore flow and fracture network flow.

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Poster / 387

Improving Colloidal Silica Grout's Performance as an Injectable Sub-surface Barrier and Soil Stabiliser for Nuclear Decommissioning

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Legacy nuclear sites typically feature subterranean volumes of radiologically contaminated soil, and concrete containment structures that have deteriorated over time. Disturbances caused by surface-level decommissioning operations exacerbate the risk of radionuclide release into the environment via contaminated groundwater. Sub-surface hydraulic barriers are needed to mitigate this, but are conventionally installed by excavation, which would require safe handling and disposal of large quantities of contaminated soil, and increase the radiation exposure of workers. Cementitious grouts can instead be injected into the ground to form barriers *in situ*, but the high viscosity of cements requires injection pressures that risk inducing ground heave, which can further damage weakened containment structures, creating additional leakage pathways. Colloidal silica (CS), however, is a novel grouting material with water-like viscosity, allowing it to be injected at minimal pressure to fill free porosity in the soil without any ground disturbance; after a time it will then transition into a rigid hydrogel with no change in volume. Unlike cement, CS is non-toxic and environmentally-friendly, has nano-scale particle size, allowing superior penetration, and has precisely controllable gelation time. CS gel's very low hydraulic conductivity facilitates its use as a hydraulic barrier, but CS also strengthens weak soils and has potential as a chemical barrier, being able to trap radioactive ions of Cs-137 and Sr-90 via chemical sorption. Additionally, CS may be suitable for other decommissioning applications, such as encapsulating radioactive waste canisters, or as a spray coating for contaminated dust.

These advantages give CS potential to make aspects of nuclear decommissioning cheaper, faster, and safer, but its application has thus far been limited. This research contributes to the case for CS's use in nuclear decommissioning by characterising the behaviour of the grout, working with industry to identify applications for it in decommissioning, and identifying ways of modifying and improving its properties to best fit these and to reduce its cost. Here, the results of compression tests are presented, showing how a range of factors and additives improve the mechanical properties of CS-grouted soil: compressive strength increases continuously with curing time, and samples cured in sea water (0.6M NaCl) are stronger than those in fresh water, with further improvement on increased concentrations and valences of salt (e.g. CaCl2). Kaolin clay additive also increases strength and may be used to partially replace silica mass to reduce cost. Combining CS with hydrophilic polymers also greatly increases flexibility. Shear vane tests show how CS is able to re-heal after damage, and pH, salinity and the presence of dissolved silica are used to enhance this. Increasing compressive strength improves CS's ability as a soil stabiliser, and increasing flexibility and re-healability gives it resistance to cracking and other damage. Ways to improve CS's water retention, hydraulic conductivity, and sorption capacity are also under investigation.

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Poster / 390

Novel multi-scale pore network modeling approach that combines high-resolution pore volume reconstruction and super-resolution segmentation

Authors: Xin Liu[1]; Viswasanthi Chandra[1]; Volker Vahrenkamp[1]

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Pore-scale studies of fluid flow in porous media are of critical importance for a wide range of energy and environmental science applications, including geological sequestration of CO2, groundwater remediation, hydrocarbon production, underground energy storage, and evaluating geothermal systems. X-ray micro-CT analysis is the most widely used method to visualize and quantify pore-scale features across multiple length scales, but poses two important challenges: first, the trade-off between sample size and resolution and second, the extremely large data size. In this study, we propose a novel pore-to-core modeling methodology that combines super-resolution and multi-scale pore network modeling that aims to address these limitations of x-ray CT scanning and improve the representation of micro- and macro-pore connectivity.

We applied the proposed method to Upper Jurassic carbonate core plugs from the Middle-East, which are representative of subsurface heterogeneity, and have bi-modal porosity distribution comprised of micro- (pore size < 10 μm) and macro-pores. First, we obtained micro-CT images of the entire core plug (one-inch diameter and three-inch long) at a resolution of 30×30×30 μm3/voxel. Guided by this overview scan, we then drilled miniplugs (0.5-millimeter diameter and one-inch long) representative of the main pore-scale rock types and obtained micro-CT images at a resolution of 6×6×6 μm3/voxel. The miniplug CT images were then segmented into micro-pore, macro-pore and solid phases under the supervision of the prior extracted from the high-resolution SEM images with a resolution of 100×100 nm2/pixel. The pair of segmented miniplug volume and the corresponding sub-volume in the full plug CT image was used to train a deep-learning network model to improve the accuracy of the segmentation of full plug CT volume. Finally, a large multi-scale pore network model of the full plug was obtained by pore network stitching (Kohanpur & Valocchi 2020), which included the macro-pore network from the full plug and micro-pore network elements reconstructed from the SEM image using multiple point statistics.

Because the training image pairs of the deep leaning network are low-resolution CT image and high-resolution segmented images, the applied of super resolution method improves the accuracy of the full plug segmentation, which is evident from the comparison of segmentation based on miniplugs. The multi-scale pore network stitching method allowed the simultaneous representation of micro-pore and macro-pore network elements while maintaining the topological features of the heterogeneous pore structures effectively. The flow property values computed from the large stitched pore network model showed significantly improved match of pore size distributions and absolute permeability values compared to lab measurements.

To the best of our knowledge, this is the first time the combination of SR-segmentation approach and 2D-3D pore volume reconstruction has been applied to generate multi-scale pore network models that are representative of micro- and macro-scale heterogeneities. The pore networks obtained from this methodology cover multiple length scale from pore-to-core and can be applied in a wide variety of pore-scale studies for multi-phase flow property predictions and simulations.

Participation:

In-Person

References:

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Implementation of a hybrid encoder-decoder structure to segment 2D micro-CT images of Sandstones

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Abstract
Reliable segmentation and identification of pore space and matrix on core micro-CT images leads to a more accurate digital rock physics characterization/analysis. Segmentation of digital images is key step for the subsequent prediction of petrophysical and fluid properties (such as porosity, permeability, fluid saturation and fluid and rock topology). There are two major categories of methods to segment 2D micro-CT images, the first one is traditional thresholding methods, and the other includes Machine Learning (ML)-based techniques. According to the recent studies, it has been proved that ML-based methods are superior to traditional thresholding due to their nature and merits like lower computational time and cost. In particular, deep learning (DL)-based techniques are often better suited to the complicated problems of segmentation of micro-CT images. As a result, the aim of this research is to present an effective hybrid DL technique and compare it with other traditional image segmentation methods. Three DL based segmentation techniques, two traditional supervised encoder-decoder structures named as U-net and Seg-Net and a hybrid structure called U-Seg-Net, are trained, validated and compared utilizing four different sandstone samples (Parker, Berea, Leopard and buff Berea sands). Parker and Leopard datasets are used for training models. For validation phase, other two samples are utilized as blind datasets. The advantages and disadvantages of each of the implemented DL-based models are carefully investigated. The results of models are compared by several validation parameters, including Intersection-Over-Union (IOU), Jaccard coefficient (JC), Precision, Recall and F1-score. Although the four sandstone data sets are completely different, our proposed model performed perfectly on all of them. Numerical value of IOU, JC, Precision, Recall and F1-score for training phase are reported as 80.18, 94.84, 99.56, 99.52 and 99.54, respectively. Consequently, it is concluded that our represented U-Seg-Net model is applicable for segmentation of rock micro-CT images and its results are applicable to properly characterize porous media parameters.

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MS06-A / 392

Micromodel of a gas diffusion electrode tracks in-operando pore-scale wetting phenomena

Authors: Anna Kalde[1]; Maren Grosseheide[1]; Sebastian Brosch[1]; Sharon Pape[1]; Robert Keller[1]; John Linkhorst[2]; Matthias Wessling[3]

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The conversion of anthropogenic CO2 emissions into valuable products in gas-fed electrochemical reactors using electricity from renewable sources is a promising solution to combat global warming. To move the chemical industry towards a closed carbon cycle, the usage of gas diffusion electrodes (GDEs) will help overcome mass transport limitations in electrochemical CO2 reduction.1[2]
Most gas-fed electrochemical reactors suffer from the flooding of GDEs within a few hours of operation, which effectively prevents stable long-term operation.[3] However, parameters which favor or prevent flooding events are not yet fully understood In addition, investigation and visualization of these parameters is challenging in conventional electrochemical reactors. In this work, we present a microfluidic model structure with multi-scale porosity featuring heterogeneous surface wettabilities to represent the behavior of a conventional GDE realistically. We establish a gas-liquid-solid phase boundary within a conductive, highly porous structure. A literature-known catalyst layer composed of silver nanoparticles and Nafion binder enables the realistic reproduction of conditions at gas-liquid-solid-interfaces seen on GDE surfaces. Especially conditions in which electrodes are partially or fully flooded can be readily investigated by our in-operando visualization method, allowing the study of wetting phenomena with confocal laser scanning microscopy. We show, that wetting of the catalyst layer is not fully reversible and demonstrate the influence of different pore sizes on GDE flooding. Application of electric potential results in the destabilization of the phase boundary and partial flooding of the electrode, thus, electrowetting is shown to have a major influence in the durability of GDEs. The influence of catalyst and binder on the advancing wetting front was investigated seperately using 3D saturation curves. This allows insights into the wetting state of electrodes based on correlations between the course of the saturation curve and the actual visualized wetting state.
Moreover, fluorescence lifetime imaging microscopy facilitates the observation of reactions on the surface of the model electrode, for the first time enabling the identification of active GDE areas, while at the same time visualizing the wetting state of the electrode. The presented results lay the foundation for the optimization of GDEs towards long-term operation of full-scale gas-fed electrolyzers.
With the aid of our microfluidic model, in-depth investigations on multi-phase wetting phenomena as well as reaction mapping are made possible, both of which are challenging or even impossible to obtain in conventional reactors. In addition, our findings may advise the design of and process

conditions for larger-scale electrochemical processes. Parts of these results were recently published by our group.[4]

Participation:

In-Person

References:

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MS09 / **393**

Numerical modeling of evaporation-condensation in nanoporous media by SPH method

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Co-authors: Magdalena Dymitrowska [2]; Amael Obliger ; Anne-Julie Tinet [3]; Fabrice GOLFIER [4]

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Extended research is necessary in view of delivering safe, sustainable and publicly acceptable solutions for the management of radioactive waste across Europe now and in the future. In light of this, a full understanding of the migration behavior of corrosion gases in clay rock environment is of fundamental importance for the reliability of scenarios predicting the long-term safety of geological repositories. The Callovo-Oxfordian clayrock, studied in France as a potential hostrock, presents the complex aspect of having a pore size distribution predominantly mesoscopic (nm), transition scale where different processes occur and interplay. Due to the low permeability of clayrock, the produced gas is expected to accumulate as a distinct gas phase which may attaint important pressure. The pressurized gas phase may desaturate the surrounding clayrock by displacement of pore water along gas flow paths, but also by the diffusion of water vapor throughout the gas phase.

In order to better understand the impact of key transport processes occurring in gas migration in clay material, pore-scale direct numerical simulations taking into account the capillary-dominated two-phase flow, the evaporation and condensation at liquid - gas interfaces, the diffusion of water vapor in

the gas phase as well as the specific feature of nanoporous materials (Kelvin effect) are proposed. The work has been carried out using the Smoothed Particle Hydrodynamics (SPH) method, a Lagrangian and meshless method which has emerged as an efficient and reliable tool for simulating complex fluid flows, like those found in porous media at the mesoscopic scale. A novel drying algorithm with Kelvin effect, which drives the local thermodynamic equilibrium between the fluid phase and the gas phase at nanoscale, has been implemented in a two-phase flow and non-deformable solid phase SPH code, initially developed at IRSN.

Different flow conditions will be first investigated for a 2D isolated pore, with and without capillary effect and/or Kelvin effect, and validated against analytical solutions. To highlight key drying behaviors occurring within pores as a function of pore geometry and throat size, we set up a series of standardized simulations over representative geometries of pore doublet. Dynamic capillary effects on pore refilling will be also discussed. Then evaporation-diffusion-condensation model will be used for simulation of drying of 2D heterogeneous pore networks. The impact of the Kelvin effect and of some dynamic capillary effects on the desaturation of the porous material will be investigated. This development should indeed serve as frameworks for upscaling. We will discuss more particularly, and compare to similar studies, the impact of drying and kelvin effect on gas drainage patterns.

Participation:

In-Person

References:

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Poster / 394

Visualization of pore formation during polymerization-induced phase separation

Authors: Sebastian Brosch[1]; Stefano Belardo[1]; John Linkhorst[2]; Matthias Wessling[3]

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Additive Manufacturing techniques become increasingly important in the fabrication of geometrically complex structures. In particular, 3D-printing allows the production of curved and overhanging geometries, which are otherwise difficult to obtain. In order to produce membranes with this degree in freedom of design, this requires the development of inherently porous 3D-printable materials.

With the principle of polymerization-induced phase separation (PIPS), porous networks can be produced from UV-active resins of different compositions.1[2] While these materials enable the fabrication of porous objects, the polymerization kinetics and the associated development of the pore system are not yet fully understood. While pore formation and phase separation phenomena were previously investigated for systems containing vesicles, nanoemulsions or colloidal gels, polymerization-induced phase separation from homogeneous solutions such as those needed for 3D-printing is not yet fully understood.[3]
In this work, a resin for porous printing was developed and modified to enable the study of pore formation by use of confocal laser scanning microscopy. Pore formation during PIPS was tracked in real-time, giving insight into the development of porosity of the printed parts. We show the different pore structures of the final cured part that can be obtained by slight alterations to the resin composition. During the PIPS process, the development of porosity and tortuosity shows distinct differences in these samples, giving further insight into the role of different components of the resins. Here, we vary the amount of porogenic solvent and are able to show, that printing times as well as pore structure are drastically influenced. Comparing the time it takes to fully 3D-print a sample object and perform detailed analysis on the final part, e.g. by electron microscopy, our method gives the opportunity to investigate small samples in a short amount of time. One measurement with our proposed method takes less than ten minutes, while a typical 3D-print of a test piece alone can take up to an hour. Thus, this technique enables rapid screening of different resins as well as furthers the understanding of pore-forming processes such as PIPS.

Participation:

In-Person

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MS06-B / 396

Mixing as restart - The role of interface shear in fluid-solid reaction efficiency under chaotic advection

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Biogeochemical reactions taking place at the fluid-solid interface in porous media are central to a broad range of natural and engineered processes. As dissolved reactants are depleted at the interface, transport limitations can limit reactant availability and reduce effective reaction rates across the plume. Reaction efficiency is thus conditioned by the mixing action of advection and diffusion. We analyze the impact of chaotic advection, which has been recently established to occur spontaneously in three-dimensional porous media [1,2], on fluid-solid reaction efficiency compared to fully-mixed conditions. The efficient exploration of the bulk of the pore space associated with chaotic mixing leads us to conceptualize excursion times [3] of solute to the reactive surface as a stochastic restart process [4], such that advecting-diffusing reactant positions are randomly restarted homogeneously across the domain over a characteristic time scale that depends on flow and geometry. Processes that restart under some condition have received much attention in the context of search strategies, where it is known that they can increase the efficiency of the underlying process. We show that flow shear at no-slip solid interfaces sets the restart rate and controls the increase of reaction efficiency with Péclet number. This has the surprising consequence that, while chaotic advection sets the stage for enhanced reaction efficiency, the increase is insensitive to the "strength" of chaos as quantified by the Lyapunov exponent. The theoretical predictions are in excellent agreement with numerical simulations of reactive decay at solid surfaces in a crystalline porous medium, over a broad range of Péclet and Damköhler numbers.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 397

Inhibiting transport of radionuclides in porous media by combining in situ electrokinetics with colloidal silica grout

Authors: Rebecca Lunn[1]; Arianna Pagano[2]; Grainne El Mountassir[1]; Andrew Cundy[3]; Frances Burrell[3]

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Nuclear energy will play a key role in the UK's strategy to achieve net zero carbon by 2050. However, the high cost and intergenerational burden of decommissioning and waste management remains high and there is a need to reduce the costs of decommissioning and clean-up. Nuclear site decommissioning involves the retrieval and handling of various radioactive waste forms. Removal of particulate wastes, such as contaminated concrete and soils, represents a potential hazard in terms of radiation exposure for the workforce and the surrounding environment. This may be due to the accidental release of airborne or groundwater-borne radioactive particulates during waste recovery and transport, or to the loss of radioactive debris upon retrieval. The development of innovative techniques to reduce hazard in decommissioning operations is therefore a critical aspect of site decommissioning.

This study explores the suitability of colloidal silica, in combination with in-situ electrokinetics, to remediate contaminated soils by promoting migration of radionuclides into grouted soil volumes, prior to their removal. Colloidal silica is an aqueous suspension of silica (SiO2) nanoparticles, with average particle size <100 nm. The creation of siloxane bonds (Si –O –Si), typically triggered by the addition of an electrolyte accelerator, leads to the formation of a solid-like network of silica nanoparticles in the form of a hydrogel. Previous work on colloidal silica gel has proved its potential to form low-permeability hydraulic barriers against fluid migration, and to inhibit the diffusion of radionuclides through the gel, making it a promising material for use in retrieval operations.

Here we present research to determine the potential for electrokinetics, in combination with colloidal silica grouting, as a low energy remediation technique for radioactively contaminated soils. Experiments were carried out using electric field gradients ≤ 1 V/cm, to satisfy the low-energy requirements that make electrokinetic remediation advantageous over other remediation methods. The effect of i) applied voltage and ii) groundwater chemistry on the mobility of two types of radionuclides, namely Cs and Sr, was assessed. These small-scale laboratory experiments demonstrate that electrokinetics can be used to mobilise radionuclides (Cs and Sr) within the ground and trap them within a relatively small volume of grouted soil that can be readily removed. As well as inhibiting groundwater flow, and thus advective migration of radionuclides in the soil, the grout also increases the sorption capacity in the ground, reduces the risk of airborne migration of radioactive particulates during excavation, and can be readily incorporated into cementitious or vitrified wasteforms.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-B / 398

Interfacial interaction of a porous periodic topology adjacent to a turbulent fluid flow by highly resolved PIV measurements

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Co-authors: Rico Poser [1]; Bernhard Weigand [1]; Grazia Lamanna [1]

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For a wide range of engineering applications such as transpiration cooling, filtration processes, heat exchangers and geothermal engineering, understanding how porous media with different topologies interact with turbulent free flows is crucial. For this purpose, the focus is on the efficient design, operation and optimisation of such engineering applications and relies on comprehensive understanding of the exchange of mass, momentum and energy across the interface between the porous medium and the free flow.

A controversial point of discussion is whether the transport at the interface is mainly diffusion or advection controlled. It is demonstrated that a viscous sublayer exists close to the permeable wall only when the intrinsic permeability of the porous medium is small compared to the viscous length scale of the fluid 1. If this requirement is fullfilled, a direct proportionality between the strain rate at the interface and the velocity difference between the interfacial velocity and the Darcy velocity inside the porous domain can be derived as an empirical boundary condition for coupling the porous media region and the free flow at the interface [2]. With the increase of the permeability Reynolds number [3] turbulent fluctuations start to penetrate into the porous media region, which is known as turbulent pumping, while simultaneously the porous media topology also affects the turbulent flow in the free flow region [4]. Due to visual accessibility inside of the porous model and the possibility of achieving high porosity, a triply periodic minimal surface topology is used as porous medium. Thus investigating both the penetration of turbulent fluctuations and the dependence of the porous media topology on the turbulent free flow is possible.

In this talk results of highly resolved PIV measurements are presented for such a porous periodic topology adjacent to a turbulent fluid flow, for both inside the porous medium region and at the interfacial region. It will be discussed (a) how the periodicity of the triply periodic minimal surface model influences the interfacial layer of the free flow, (b) how the flow field behaves inside the periodic porous region and (c) which flow phenomena occur at the interface of the porous medium and the free flow, specifically emerging vortices.

Participation:

In-Person

References:

1 S. Hahn, J. Je, and H. Choi. Direct numerical simulation of turbulent channel flow with permeable walls. Journal of Fluid Mechanics, 450:259 –285, 2002.

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399

Coupled Geochemical-geomechanical Processes in CO2 Sequestration Reservoirs in Southeast, US

Authors: Zhuofan Shi[1]; Jack Montgomery[1]; Charlotte Garing[2]; Lauren Beckingham[1]

[1] *Auburn University*

[2] *University of Georgia*

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Geological CO2 sequestration is currently one of the promising solutions to mitigate atmospheric CO2 and to minimize climate change. When CO2 is injected and dissolves into formation brine, the brine pH becomes lower. These acidic conditions can be highly geochemically reactive for the minerals in the storage reservoir. CO2 induced mineral reactions may alter the transport and mechanical properties of the formation, impacting injectivity and reservoir security. It's important to understand how fast the reactions are and the impact of reactions on formation properties. The present study investigates mineral dissolution rates and changes in porosity, permeability, and stiffness in core samples mimicking CO2 sequestration systems in southeastern United States. Representative sandstone samples were tested in this study and implications for SE regional storage formations considered. We conducted core flood experiments in a custom-built triaxial core holder equipped with in-situ acoustic transducers at a temperature of 50˚C and pressure of 100 bar. During the experiments, the differential pressure across the core was continuously monitored and used to infer changes in the permeability of the core sample due to mineral reactions. The aqueous effluent samples were periodically collected, and their composition were measured using ion chromatography. Ion concentrations were used to infer column scale mineral dissolution rates and the evolution of mineral volume fractions. Changes in the material stiffness were detected via acoustic wave velocities. These changes in stiffness can be correlated to changes in the mineral volume fractions and degradation of sample cementation. Before and after the experiments, 3D images of the core samples were captured via 3D X-ray Computed Tomography to determine the changes in porosity, pore connectivity, and the evolution of mineral surfaces.

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References:

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Energy Transition Focused Abstracts:

MS15 / **400**

Fast Physics Informed Surrogate Models for Fluid Flow in Porous Media: Learning Operators using DeepONets

Author: Waleed Diab[1]

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Corresponding Authors: mohammed.alkobaisi@ku.ac.ae, 100049411@ku.ac.ae

Simulating fluid flow in reservoir models is an expensive and time-consuming task. Given the inherent uncertainty in most measurements used as inputs for these models, it is customary to perform stochastic modeling in order to reduce and quantify the uncertainty. Recently, a new class of machine learning algorithms referred to as operator learning has been developed. These algorithms, such as DeepONets and Fourier Neural Operators, can learn mappings between two infinite-dimensional spaces. However, these approaches suffer from data inefficiency as they require thousands of training observation pairs in the input and output domains which is computationally prohibitive. Physics-informed DeepONet has been proposed as a remedy to this problem. In this paradigm, DeepONets are regularized by underlying physical laws in a manner similar to Physics Informed Neural Networks (PINNs), hence the name. Physics-informed DeepONets can learn the solution operator mapping between a set of initial and boundary conditions to the full spatio-temporal solution making it a powerful tool for parametric PDE learning. Here, we investigate the applicability of Physics-informed DeepONets to an immiscible two-phase fluid flow problem through a 1D porous medium. We provide two test cases. First, we attempt to learn the solution operator mapping of an initial condition to the entire spatio-temporal solution of all possible initial conditions. Second, we test Physics-informed DeepONets to learn the solution operator mapping of a boundary condition to the entire spatio-temporal solution of all possible boundary conditions. Our results show that with a small sacrifice in accuracy, enormous gains in speed can be achieved, as this approach can solve thousands of PDEs in a fraction of a second.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 402

Pore-scale investigation of gas mixing, brine salinity, and salt type influence on the dynamic contact angle using Microfluidics for underground CO2 sequestration

Author: Amer Alanazi[None]

Co-authors: Abdullah Bukhamsin ; Saleh Bawazer [1]; Muhammad Ali [2]; Hussein Hoteit [3]

[1] *Assistant professor at College of Engineering and Islamic Architecture, Umm Al-Qura University*

[2] *King Abdullah University of Science and Technology*

[3] *King Abdullah University of Science & Tech (KAUST)*

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Geological storage of hydrogen (H2) and carbon dioxide (CO2) is pivotal for a successful energy transition toward a diversified low-carbon economy and a net-zero emission future. Wettability of reservoir rocks in the presence of formation fluids and H2 or CO2 is a controlling factor of gas mobility, residual trapping, and efficient storage. However, the influence of different brine types (salt type and concentration) and gas contamination on wettability is rarely reported in the literature.
Therefore, this paper presents the results of a set of experiments using a microfluidic chip of different diameters (50, 70, 90, 110, and 130 μm) measuring CO2/brine and N2/brine advancing, receding, and static contact angles for different brine types and mixing ratios (10%, 30%, and 50%) at constant conditions (P=14.7 atm and T= 22 ℃). The experiments were conducted using a constant brine rate at 0.1 μL/min during imbibition. A sophisticated Matlab code was built to measure contact angles from live videos of the microchips, allowing the generation of multiple data points with controlled upscaling.
The measurements indicate the channels are strongly water-wet for all the tested brine with CO2. The advancing and receding contact angles vary from 9.5° to 38° and from 6.5° to 29°, respectively. The contact angles slightly increased with increasing brine salinity varying between the different types of salt (NaCl, MgCl, and KCl). The MgCl2 demonstrated the highest values of contact angles. The contact angles increased with increasing the mixing ratios between CO2 and N2 from 10% to 50% and decreased with channel diameters. Higher hysteresis was observed with a higher mixing ratio indicating a significant impact of contamination on the storage process.
The presented experimental approach depicts a time-effective technique to investigate crucial influencing parameters using microfluidic chips for effective and successful underground CO2 sequestration.

Participation:

In-Person

References:

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MS09 / **403**

Turbulent transport across the sediment-water interface: Pore-resolved direct simulations and upscaled modeling

Authors: Shashank Karra[1]; Sourabh Apte[1]

[1] *Oregon State University*

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Pore-resolved direct numerical simulations (DNS) are performed for turbulent open channel flow over a randomly packed porous sediment bed over a range of permeability Reynolds numbers of

$Re_K = \mathcal{O}$(1-10) representative of aquatic systems. A fractional time-stepping based fictitious domain method (Apte et al. 2008) is used to simulate flow over spherical sediment particles on Cartesan grids by enforcing the rigidity and no-slip condition on the particle boundaries. The DNS predictions are compared with the experimental data of Voermans et al. (2017) to show excellent agreement of mean and turbulent flow quantities. A space-time averaging methodology is used to compute the Reynolds stresses, form-induced stresses, and pressure fluctuations. Shear layer and turbulent shear stress as well as Reynolds and form-induced bed-normal stresses increase with Re_K. The peak values of the form-induced stresses were found to occur within the top layer of the sediment bed for the Reynolds numbers studied. The sum of turbulent and form-induced pressure fluctuations at the zero-displacement planes are statistically similar and can be well approximated by a $t-$ location-scale distribution fit based on high-order statistics, providing with a model that could potentially be used to impose boundary conditions at the SWI in reach scale simulations. A continuum model based on the volume-averaged Navier-Stokes (VANS) equations is developed by defining smoothly varying porosity across the bed interface and modeling the drag force in the porous bed using a modified Ergun equation with Forchheimer corrections for inertial terms (Wood et al., Annual Review of Fluid Mechanics, 2020). A spatially varying porosity profile generated from the pore-resolved DNS is used in the continuum approach. Mean flow and Reynolds stress statistics and net momentum exchange between the free-stream and the porous bed are compared to show very good agreement. The continuum VANS approach allows for significant reduction in computational costs, thereby allowing to study hyporheic exchange of mass and momentum in large scale aquatic domains with combined influence of bedform and bed roughness.

Funding from US Depart of Energy, Office of Basic Energy Sciences (Geosciences) under award number DE-SC0021626, Pacifict Northwest National Laboratory's internship program, as well as US National Science Foundation award \#205324 are gratefully acknowledged.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 404

Characterising the development of fungal networks in complex porous media

Authors: Qi Zhang[1]; Grainne El Mountassir[1]; Alireza Fathollahi[1]

[1] *University of Strathclyde*

Corresponding Authors: alireza.fathollahi@strath.ac.uk, qi.zhang@strath.ac.uk, grainne.elmountassir@strath.ac.uk

Fungi are the largest source of biomass within soils, yet fungi are frequently neglected within the environmental microbiology and environmental science research disciplines (Gadd et al., 2007). Fungi are known to play vital roles in soils: as symbionts with plants, as decomposers and in elemental cycling. Furthermore, basidiomycota fungi have been shown to successfully degrade organic contaminants in soils (Bezalel et al., 1996) and more recently have been proposed as a novel nature-based solution within the field of ground engineering (El Mountassir et al., 2018; Salifu et al., 2022).

One of the significant challenges in the deployment of fungi within civil and environmental engineering applications is the ability to understand, control and optimise the growth of fungal networks. To date, much of the work on fungal-soil interactions has been carried out in 2D systems where growth of the fungus/fungi is promoted to occur at the soil-air interface by compaction of soils. This study investigates the 3D fungal networks that are created within complex soil media (solid soil particles, carbon substrate, air and liquid phases) by also considering fungal growth with depth into soils.

A series of column experiments were conducted investigating the ability of various UK native basidiomycota species to grow with depth. Nutrients were emplaced in varying spatial arrangements within the soil. A methodology was developed in this study to characterise the fungal networks developed within the soil by: staining fungal hyphae, preparation of resin impregnated soil samples, optical microscopy and image analysis. Biochemical analysis was also carried out to determine hot water extractable carbohydrate as an indicator of microbial biomass with depth. The development of this methodology to characterise fungal networks allows us to more readily understand differences in growth behaviour between different fungal species and the differences in mycelia architecture that can exist with depth. This will be of critical importance for identifying fungal species that have the potential to be applied at larger-scales both for ground and environmental engineering applications.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS13 / 405

Surface interactions and reactions strongly impact ion adsorption and electrokinetic transport

Author: Remco Hartkamp[1]

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Corresponding Author: r.m.hartkamp@tudelft.nl

Detailed insight into the structure and electrokinetic transport of electrolyte solutions in nanoconfinement is hard to obtain. Experimental techniques are often either limited in their accessible resolution or their interpretation relies on models and assumptions that may not hold in nanoconfinement. Molecular simulations can in principle provide such insights, but the simulation results depend sensitively on the model input. Consequently, both the experimental and computational literature contains various contrasting data.

In my talk, I will focus on two aspects of simulating nanoconfined electrolytes. First, I will present an effective method to use unambiguously interpretable experimental data to tune simulation input and I will use these simulations to provide new insight into the coupling between ion adsorption and transport 1.

Second, I will present a method that allows the surface charge distribution on a non-conducting material to evolve in time, thus mimicking the effect of surface reactions in chemical equilibrium [2]. Such reactions are universally assumed to have no notable influence on interfacial fluid properties, regardless of the simulation time, surface material, or temperature considered. Our simulations show that accounting for surface reactions can strongly and qualitatively affect ion adsorption and electrokinetic properties.

Participation:

In-Person

References:

1 M.F. Döpke and R. Hartkamp, "The importance of specifically adsorbed ions for electrokinetic phenomena: bridging the gap between experiments and MD simulations" J. Chem. Phys. 154 094701 (2021)

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Energy Transition Focused Abstracts:

MS09 / 406

Stochastic Methods for the Generation of Granular Porous Media with Conditional Heterogeneity

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Understanding the mechanical behavior and fluid flow properties of porous media composed of packed particulate has numerous applications within the physical sciences and engineering, being pertinent to the study of naturally occurring geo-materials, such as sedimentary rocks, and engineered media, such as fuel cells and catalysts. Both manmade and geologic granular porous media often exhibit pronounced spatial variability in their component particle sizes, which in turn, imparts internal heterogeneities in porosity, permeability, capillarity and mechanical strength within the particle column. Numerical methods for the simulation of pore-scale fluid flow or granular mechanics (e.g., Lattice-Boltzmann, finite volume and discrete element methods:) have enjoyed widespread application over the past decade, owing to the proliferation of both commercial software and open-source libraries through which such models can be readily deployed. Coupled with advances in volume imaging of real porous media (i.e., x-ray microcomputed tomography), workers are now able to probe such processes numerically within highly heterogeneous pore networks, providing a wealth of insights into the key physical properties of a wide range of porous materials [e.g., 1-3]. Despite these developments, objective methods for the generation of synthetic porous media characterized by grain-scale heterogeneities in particle size, mirroring those observed in both naturally occurring and manmade porous materials (i.e., layering, grading, lenses, nested pore structures / intragranular and matrix porosity) remain limited. The availability of such a framework is conceptually attractive, as it provides the means to introduce conditional heterogeneity into computational fluid dynamics and discrete particle scale mechanical simulations, providing experimental control over spatial variability in particle size for such studies.

In this work, we present a method capable of simulating granular media which can represent pore-scale heterogeneities commonly observed within a wide variety of natural (i.e., geologic) and manmade porous materials alluded to above. Here, we utilize a modified implementation of the sequential deposition algorithm from the classic material physics literature towards the generation of highly heterogeneous 2D and 3D particle beds (sphere packs), amenable to computational fluid dynamics (CFD) and the initialization of discrete element model (DEM) based mechanical simulations. The presented approach utilizes closed form analytical solutions for the detection of linear and rotational collision between the mobile and static particle pack, meaning that it is computationally efficient and amenable towards the generation of granular porous media containing large numbers of elements. We demonstrate the power of the approach using finite volume CFD simulations of immiscible fluid flow using a range of heterogeneous pore systems generated using our novel framework.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

407

Microwave-assisted synthesis of calcium oxide microstructures for carbon dioxide capture at high temperature and moderately high pressure

Authors: Paola Arjona-Jaime[1]; Rene Rangel-Mendez[1]

[1] *Instituto Potosino de Investigación Científica y Tecnológica, A.C. (IPICYT)*

Corresponding Authors: rene@ipicyt.edu.mx, alejandra.arjona@ipicyt.edu.mx

Carbon dioxide (CO₂) had contributed more than 66% to global anthropogenic greenhouse gases (GHG) emissions since the preindustrial era, resulting in the current climate crisis (1). The global CO₂ emissions from the burning of fossil fuels increased about 6% in 2021 compared to 2020, reaching 415.7 ppm in 2021 (1,2). In this way, carbon capture, storage and utilization technologies have been proposed to mitigate the CO₂ accumulation in the atmosphere. Alkaline earth metal oxides, as calcium oxide (CaO), have been proposed as sorbents of CO₂, where 1 mol of CaO chemically interacted with a stoichiometric equivalent of CO₂ to form a calcium carbonate (CaCO₃) (3). However, its main drawback is the low cyclic stability due to sintering, altering the morphology and the CO₂ sorption capacity in the first 20 cycles of carbonatation-calcination (4,5). The synthesis of micro and nanometer sized CaO particles has been proposed to reduce the sintering decay and increase both the dispersion between particles and the external surface area (6). The synthesis of CaO particles and Ca(OH)₂ precursor has been studied through different processes as chemical precipitation, thermal decomposition, sol-gel and hydrothermal processes (7). However, the microwave-assisted synthesis has shown advantages due to its simplicity, time, reproducibility, and energy efficiency. In addition, it has shown an interesting control over the morphology and size of particles due the rapid and homogeneous heating by microwave irradiation, a result of the collision and reorientation of charged particles. However, this technic has not been reported, to the best of our knowledge, for the development of CO₂ sorbents (8–11).
In this work, Ca(OH)₂ was obtained by microwave-assisted synthesis, using Ca(CH₃COO)<s
and NaOH as precursors. The synthesized conditions over the precipitate recovery and the particle size were evaluated with a central composite design. After the Ca(OH)₂ calcination at 750 ℃, CaO microstructures with particle sizes >1 μm were obtained. The formation of CaO was confirmed by FT-IR, XRD, TGA-DTA and DLS techniques. The calcium-based sorbents showed potential for CO₂ capture at high temperatures, with capacity values of 13.82 mmol/g at 875 ℃, until the CaCO₃ formation. Moreover, CaO sorbents exhibited an enhanced reversibility of more than 90% at moderately CO₂ high pressure (8 bar), suggesting a superficial interactions between gas-CaO and CO₂-CO₂ molecules. Multiple operation cycles of CO₂ capture at different temperature and pressure are currently being conducted to evaluate the use of CaO microstructures in post combustion capture systems.

Participation:

Online

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Poster / 409

Pore-scale investigation into dynamics of salt crystal nucleation, precipitation and growth in porous media during CO2 sequestration in saline aquifers

Authors: Mohammad Nooraiepour[1]; Mohammad Masoudi[2]; Helge Hellevang[3]

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In a full-scale CCS, millions of tons of CO2 must be stored underground. Injection of dry or undersaturated (with respect to water) CO2 leads to dry-out of the brine formation water and salt precipitation, particularly in the near wellbore region, causing reduced injectivity and deteriorated reservoir rock properties. We report a series of microfluidic experiments on glass- and geomaterial (real rock) microchips representing matrix and fractured systems to provide insights into some

open questions regarding the pore-scale physics and dynamics of CO2-induced salt nucleation, precipitation, and growth in porous media. The study is complemented with LBM reactive transport simulation of nucleation and growth to further elucidate the evolution dynamics from precipitation of single crystal to eventual clogging of flow pathways. The results introduce two interrelated phenomena –self-enhancing of salt growth and water film salt transport, which together remarkably intensify the rate and amount of precipitations. It is shown that salt crystals, although at different rates, grow in both aqueous and gas phases. The pore-scale observations indicate that the trapped water films in porous or fractured media have enough continuity and conductivity to transport residual brine to an evaporating front and cause an increase in the rate and amount of precipitated halite crystals. The results also indicate that CO2 phase states and pressure-temperature conditions control the magnitude, distribution, and precipitation patterns of salt precipitates. Injection of gaseous CO2 resulted in higher salt precipitation compared to liquid and supercritical CO2. The thermodynamic conditions influence salt precipitation via water solubility in CO2, maximum water flux into the CO2 stream, and balance between the imposed viscous forces and capillary-driven backflow. The mutual impacts of the continual growth of salt crystals toward the injection point, the affinity of salt bodies to become connected, access to brine pools via conductivity of water films, porous structure of many salt bodies, imposed capillary suction towards the evaporation front, concentration gradients, in addition to the extent of CO2-induced salt accumulations suggest that the salt precipitation during injection of CO2 into the geologic formations can be a critical phenomenon with a complex interplay on coupled THMC processes. The research outcome highlights processes and dynamics crucial to consider when investigating salt precipitation induced by CO2 injection, as this phenomenon has implications for injectivity and containment. For better reservoir-scale numerical modeling, such mechanisms must be incorporated and scaled up in the reservoir simulator, along with a representative physically-sound scale-aware clogging model. We provide insights into the applicability of present clogging models and porosity-permeability relationships for predicting dynamics changes induced by solid accumulation in pore space. Present-day reservoir-scale simulators of salt precipitation consider mechanisms such as water evaporation into CO2 and capillary backflow of water into the dried zone, suggesting only a limited impact on the porosity and permeability. Additionally, the current approach for modeling salt precipitation using the volumetric method in the reservoir-scale numerical simulator may not reflect the required physics for investigating salt precipitation induced by CO2 injection.

Participation:

In-Person

References:

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Masoudi, M., Fazeli, H., Miri, R., Hellevang, H., 2021. Pore scale modeling and evaluation of clogging behavior of salt crystal aggregates in CO2-rich phase during carbon storage. Int. J. Greenh. Gas Control 111, 103475. https://doi.org/https://doi.org/10.1016/j.ijggc.2021.103475

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MS11 / 410

Pore-scale visualization of emulsion flow in linear and radial microfluidic porous media

Authors: Clarice de Amorim[1]; Amanda da Costa e Silva de Noronha Pessoa[None]; Ranena V. Ponce F.[1]; Marcio Carvalho[1]

[1] *PUC-Rio*

Corresponding Authors: amanda.pessoa@lmmp.mec.puc-rio.br, msc@puc-rio.br, poncerv@lmmp.mec.puc-rio.br, camorim@lmmp.mec.puc-rio.br

Pore-blocking efficiency is a key factor when dilute and stable emulsions are used as flow diversion agents to increase oil recovery and reduce water mobility in preferential flow paths. Emulsion plugging occurs when droplets of the dispersed phase are trapped in the pore throats as they flow through porous media. The droplet capture phenomenon is highly dependent on the drop-to-pore size ratio, the dispersed phase concentration, and the capillary number. Therefore, understanding the transport of droplets and the physical mechanisms of pore-blocking at the micro-scale is fundamental for a proper design of emulsion flooding as an enhanced oil recovery (EOR) method. The performance of oil-in-water (O/W) emulsions as pore-blocking agents was investigated by studying the transport of oil droplets through transparent porous media. To this end, a 2D PDMS/glass porous media micromodel with varying constriction sizes was used. O/W emulsion systems with two distinct drop size distributions were formulated to conduct the tests at different capillary numbers. The tests were performed by recording the injection pressure response during the sequential flow of an aqueous phase, followed by emulsion (oil drops dispersed in the aqueous phase) and then by a second slug of the aqueous phase. The association of microfluidic devices and imaging techniques provided a robust methodology, combining accurate pressure measurements and pore-scale visualization of the droplets'capture phenomenon during emulsion flooding. Detailed visualization of the flow was achieved by high-speed image acquisition at different stages of the test to identify the droplets'capture mechanisms and their capture/release dynamic in the pore throats. Droplets larger than the pore constrictions were captured by the straining mechanism, while the smaller ones were adsorbed on the pore walls, blocking the flow paths by droplet accumulation (bridging). At low capillary numbers, a larger number of droplets were captured in the pore throats because of the stronger capillary forces. As the capillary number was increased above a threshold value, the viscous force was large enough to overcome the capillary resistance and the droplets were able to deform and re-enter the flow stream. This behavior was quantitatively demonstrated by comparing the mobility of the emulsion to that of the aqueous phase. Finally, a pore-scale visualization study was also conducted in a radial porous media micromodel to evaluate the performance of emulsion flooding with varying capillary numbers. The relationship between mobility control and the capillary number was investigated aiming to define the desired location of the pore-blocking.

Acknowledgments
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In-Person

References:

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Energy Transition Focused Abstracts:

MS08 / **412**

How probabilistic nucleation controls spatiotemporal dynamics and dimensionality of mineral growth in porous media?

Authors: Mohammad Nooraiepour[1]; Mohammad Masoudi[2]; Helge Hellevang[1]

[1] *University of Oslo, Norway*

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Precipitation and growth of solid phases during a reactive fluid flow and solute transport are critical in many natural and industrial systems. Mineral nucleation and growth is a prime example where (geo)chemical reactions give rise to geometry evolution in porous media. The precipitation reactions can reduce the amount of void space, alter pore space connectivity and morphology, modify tortuosity, deteriorate permeability, and change the fluid flow and solute transport. Additionally, precipitation events reshape the available surface area for growth, leading to changes in reactivity, reaction progress, and reaction rates. The target is to ideally limit the mineral growth in many applications, such as avoiding damage to reservoir permeability due to solid precipitation near CO2 injection wells. In other cases, maximizing mineral growth in porous media can be highly favorable, such as sealing fractured caprocks or increasing mineral trapping in the sequestration sites. Understanding, controlling, and predicting this reactive transport phenomenon is challenging because it requires coupling flow, transport, and chemical processes often characterized by different temporal and spatial resolutions. Nucleation is the pre-growth process that controls the primary position of any mineral precipitation and subsequent growth dynamics. Mineral nucleation is a probabilistic process where crystals might nucleate anywhere given similar conditions, such as surface properties, supersaturation, and temperature. It is imperative to use a probabilistic approach or an upscaled physically sound representation to understand the effect of mineral precipitation on porous medium hydrodynamics. Motivated by the importance of incorporating stochastic dynamics of nucleation and growth kinetics in studying various multiphase and multiscale processes occurring in geo-environmental and geo-energy systems, this paper provides numerical and experimental insights into the recently proposed probabilistic nucleation model. We present laboratory experiments (microfluidic and flow-through column reactor) and pore-scale reactive Lattice Boltzmann Method (LBM) numerical simulations. As variations in the properties of the porous medium are intimately linked to the spatial distribution of the precipitation events, we quantify the evolution of experimental and numerical modeled systems at different physiochemical conditions by mapping the disorder of the system (Shannon's entropy) induced by the spatial mineral distributions across time. We use experimental and numerical results to show the importance of the spatial and temporal location and distribution of nucleation and growth events, particularly when the interplay among several determining parameters is inevitable. The results show that probabilistic nucleation contributes to broad stochastic distributions in both amounts and locations of crystals in temporal and spatial domains.

Participation:

In-Person

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MS09 / **413**

Analysis of capillary pumping during the drying of heterogeneous porous media using Lattice Boltzmann modelling

Authors: Linlin Fei[1]; Dominique Derome[2]; Jan Carmeliet[3]

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The drying of heterogeneous porous materials is accompanied by capillary pumping from large to small pores which results in the surface remaining partly wet, guaranteeing an almost constant drying rate. At certain degree of saturation, the capillary pumping is turned off and the material experiences a decreasing drying rate. A two-component two-phase Lattice Boltzmann model 1 is used at pore scale to simulate the convective drying process of a dual porosity layered porous material showing the influence of inflow air speed (Re number), inflow vapor concentration difference from the liquid-vapor interface and contact angle. Using these parameters, a universal scaling law is derived which allows predicting the drying rate during the constant drying period [2].

The conditions for capillary pumping are derived based on simulation of the drying of a system of two (and four) connected channels of different size. Sequential drying of the channels from large to small guarantees a maximal drying rate, and is controlled by the capillary pressure difference between the channels and the fluid permeability of the connecting pores. An analytical model at pore scale is developed based on this interaction between capillary channels where the drying across the boundary layer is modelled with a mass transfer coefficient. This analytical model is applied to the drying of real porous materials, like ceramic brick and calcium silicate stone. The former material shows from start a high drying rate and dries out over several days, while the second material needs hundreds of days to dry. Using the developed drying model and a known pore size distribution, the drying curve for these two materials can be predicted with good agreement. Finally, we use this new model as a toy model to design the pore structure of materials to meet expected drying patterns, showing that the presence of well-connected coarse pores of different sizes promotes a fast drying of porous materials.

Participation:

In-Person

References:

1 Linlin Fei, Feifei Qin, Jianlin Zhao, Dominique Derome and Jan Carmeliet, Pore-Scale Study on Convective Drying of Porous Media, Langmuir, vol. 38: no. 19, pp. 6023-6035, Washington, DC: American Chemical Society, 2022. DOI: 10.1021/acs.langmuir.2c00267

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Energy Transition Focused Abstracts:

Poster / 414

Water permeability reduction associated with injection of oil-water emulsions and microcapsule suspensions in Bentheimer sandstone

Author: Paulo Hoyer[1]

Co-authors: Lisbeth Manchego [2]; Jorge Avendaño [2]; Marcio Carvalho [1]

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In recent years, water alternate emulsion injection (WAE) has been explored as a potential enhanced oil recovery method. Emulsion drops may block the pore throats diverting the aqueous phase towards oil-containing pores. The efficiency of the method strongly depends on the drop size distribution and interfacial properties of the emulsion. Emulsions are thermodynamically unstable systems and their characteristics can be affected by various reservoir conditions such as temperature, salinity, and surfactant adsorption on the rock walls.

The alternative explored in this work is the use of a dispersion of microcapsules with a biopolymer (gellan gum) thin shell as an alternative to emulsions. Microcapsules, which can also block throats in the porous medium and produce the same positive damage effect as emulsions, are less susceptible to reservoir conditions since their shell acts as a physicochemical barrier against coalescence and drop breakup during flow through the pore space. Moreover, the mechanical properties of the microcapsule shell can be adjusted by changing the polymer structure, leading to different flow resistance.
To compare the mobility reduction caused by the dispersed phase of an o-w emulsion and a microcapsule suspension with the same diameter distribution, we performed experiments using a miniaturized Bentheimer core, which allowed faster parametric analysis of the effect of different parameters on the flow behavior. The pressure difference was monitored during the injection at constant flow rate of slugs of the water, followed by a slug of the dispersion (o-w emulsion or microcapsule suspension), followed by a second slug of water. The ratio of the water permeability between the first and second water slug was evaluated as a function of drop size distribution and shell properties. The results reveal the optimum microcapsule properties to achieve a desired mobility reduction.

Participation:

In-Person

References:

Oil-water emulsion; microcapsule suspension; permeability reduction;alternate emulsion injection (WAE); enhanced oil recovery (EOR); core flooding; Bentheimer Sandstone;

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Energy Transition Focused Abstracts:

MS19 / **416**

Reflection and Transmission Coefficients at the Interface of Fluid-Saturated Porous Media

Author: Fabien Borocin[None]

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We consider a classic problem of acoustic waves reflection at the interface between two visco-poroelastic saturated materials.

Decomposing the wavefield into downgoing and upgoing plane waves, we write down explicitely the polarisations for all waves (P-, Biot-, Sv- et Sh-waves). In analogy with the elastic case, the reflection-transmission-conversion (RTC) coefficients can then be obtained as a function of frequency and incidence angle 1. With a simple matrix form, the algorithm presented is suitable for conventional computations of multilayered stacks.

For low frequencies, an analytic approximation is derived for RTC coefficients at normal incidence. Contrary to a usual assumption found in the literature [2], numerical simulations show that the second-order term in (square-root of) frequency cannot always be neglected.
In particular, it is shown that this leads to a quasi-linear behaviour of the RTC coefficients in the range of seismic frequencies and values of parameters typical of marine poroelastic sediments.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-A / 417

A Thermodynamically Consistent Model for Compositional Multiphase Flows

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While irreversible thermodynamics has proven his relevance in modelling of flows through porous media, explicit and usable formulations based on thermodynamics remain few and hard to extend. Yet thermodynamics offers powerfull concepts to achieved the coupling of the wide variety of processes occuring in porous media. This work proposes to apply the principles of irreversible thermodynamics to compositional multiphase flows through porous media and to derive from them a formulation that encompasses the most usual models.

Starting from a clean decomposition of the porous media system between the volume of matrix, the volumes of fluids and the interfaces, the entropy is assumed to be a Euler homogeneous function of first order of the total internal energy, the total mole numbers of each component, the volumes of each fluid, the areas of each interface. The entropy balance equation is then derived from the energy and mole balance equations.

The local entropy production brings out a term that summarizes the exchanges of mechanical work between fluids and interfaces. Such a dissipation term, counting for the interface displacements and deformations, gives a proper definition for the interface equilibrium assumption : interface dissipation is zero, interface transformations are reversible. We show how that interface equilibrium assumption is fundational for the common idea of capillary pressure curve. Indeed, it appears that all the capillary pressure curves in a given porous media derive from a unique convex potential. Although the two phase case is trivial, for three and more phases, this result is strongly structuring, possibly conflicting with some capillary models proposed in the litterature.

The other entropy production terms are related to energy and mass transfers. They come in the form of flow-force products and are compatible with usual laws like Darcy's law for the fluid velocities and Fourier's law for the thermal conduction. The exception is the molecular diffusion where the more classical Fick's law (driven by the gradient of concentration) is not compatible with the positivy of entropy production expected by the second principle. Instead, we have to consider generalizes Fick's laws or Maxwell-Stefan diffusion that are driven by the gradients of the chemical potentials.

In order to ensure the usability of such of modeling, we conclude by proposing a closed formulation, based on a fixed set of primary variables related to the temperature and the chemical potentials. The data of the model are the coefficients for flux-gradient laws, the equations of state for the fluids and the "capillary" potential. The total entropy of the local system is provided and the entropy balance equation derivation is natural thanks to the choice of primary variables.

Participation:

In-Person

References:

Smaï, 2020. A thermodynamic formulation for multiphase compositional flows in porous media (preprint) - https://hal.archives-ouvertes.fr/hal-02925433v1

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Energy Transition Focused Abstracts:

Poster / 418

Flow of a fluid with pressure-dependent viscosity through aging porous media

Author: Shriram Srinivasan[None]

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Considerable experimental evidence in a variety of porous materials (concrete, ceramics, bones, rocks) that undergo infinitesimal deformations makes it clear that material moduli depend on the density (identified as density dependence of Young's modulus).
The phenomean of material damage is a consequence of the inhomogeneity of the body as material properties detieriorate with deformation.
This is especially relevant for subsurface flows through geological media which have experienced deformation over millenia.
However, the most widely used models for subsurface flow (such as Darcy/Brinkman model) typically assume that the porous medium is a rigid skeleton. Even if one moves onto theories of poroelasticity, the porous solid is assumed to be a linearized elastic solid with constant values of material properties such as Young's modulus.
Within the framework of linearized elasticity, modelling damaged porous media with a density dependent Young's modulus is inconsistent and untenable due to the assumption of infinitesimal displacement gradient. However, it is possible to incorporate density-dependent material moduli in the framework of implicit constitutive theories where the kinematic variable (strain) is expressed as a function of the stress.
Such a viewpoint remains unexplored in the context of flow of a fluid through porous media, and we shall
illustrate the effect of damage by comparison with existing theories that ignore it completely.

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Simulation of the two phase displacement characteristics in porous media based on the digital core technology

Authors: Dong Wang[None]; Jiaqi Liu[None]; Yingge Li[None]; Dongxing Du[None]

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Reservoir evaluation is essential for oil and gas exploration and development. In order to revealing the mechanisms behind the oil recovery enhancement practices, the pore scale investigations on multiphase displacement behavior with help of digital core technology have attracted lots of research interest.
In this paper, the two phase displacement behavior in the porous media were studied on the pore scale. Digital rock technology was employed to reconstruct successfully the complex pore structures in the rock. Then the single-phase flow characteristics, including the velocity and pressure distribution, were investigated to validate the methodology. Then the water displacing oil process in the porous media was scrutinized with help of the state-of-the-art Computational Fluid Dynamics (CFD) software of Fluent. The Mixture model was employed to simulate the two phase flow process and three key influential factors, including interfacial tension, wettability and displacement pressure, on oil displacement efficiency are numerically studied.
In the single phase simulation case, the seepage characteristics of the fluid flow in porous media is studied, and the results show the complex and changeable orifice-throat flow channel results in non-uniformity and changeability of flow. The obtained rock absolute permeability agrees perfectly well with the measurement result, which validates the methodology employed in this paper. In the water displacing oil simulation cases, parameter studies on three influencing factors indicate that displacement pressure is the most direct factor affecting displacement efficiency, while interfacial tension is an important factor hindering flow, and the favorable water wettability can effectively improve displacement efficiency. In summary, the methodology described in this paper could reproduce transport characteristics in porous media in the pore scale, analyze important effective physical parameters, and therefore provides an accurate and effective alternative method for reservoir research and evaluation.

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Energy Transition Focused Abstracts:

MS21 / 420

Non-linear flow phenomena in a porous cylindric microtube

Authors: Florian Cajot[1]; Philippe Beltrame[2]

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The understanding of water transfer in heterogeneous porous media such as soils is at the center of many issues such as water resource management. In the macroporosity as opened cracks, earthworm burrows free surface flow can be a dominant (Sammartino et al., 2012). Very little is known about the physical processes involved in infiltration, whether it is the form of streamflow, continuous films in the macropore (Keven and Germann, 2013) or the "active" macroporosity during a flow and also the exchange mechanisms at the macropore interface (Katuwa et al., 2015). Answering these questions on a small scale is crucial because, for example, the filling rate of a macropore is closely related to colloid filtering, water retention phenomena. The last decades many models have been developed to model flow in macroporosity such as dual porosity with Kinetik Dispersive Waves models (Di Pietro et al., 2013) or conceptual approaches to film flow as in Nimmo et al. (2010). However, these models still do not explain all of the observed flows made by imaging techniques (Sammartino et al., 2015 ; Lissy, 2019).

In this paper, we focus on the modelling and simulating free surface flow in a cylindrical microtube taking into account the physicochemical properties of the matrix and at the interface between the matrix and the macropore. Indeed, organic matter is known to generally impart hydrophobic properties to soils. In an impervious microtube surface, a rich range of flow shapes has been identified: droplets, thin films or rivulets and notably, there is a regime leading to complete wetting (Beltrame, 2018). In the present work, the mesopore surface is porous and fluid transfer may appear through the interface between the macropore and the soil matrix.

The model is based on the long-wave approximation with a free surface. The soil matrix wettability is taking into account using disjoining and conjoining pressures as presented in Beltrame (2019). The linear classical flux condition on the liquid/porous interface as used in Ding and Liu (2011) does not yield if a hydrophobic coating is present: the flux depends on the matrix moisture too (Doerr et al., 2000). Our present model takes into account wettability at the surface and also in the porous matrix (Beltrame and Cajot, 2022). Thus, the dynamics, both in the matrix and in the macropore, are governed by a gradient type equation (Thiele, 2018) where free energy terms characterize the wettability.

Using numerical simulation and bifurcation diagrams, a rich behavior is brought to light. Notably, several flow regimes in a microtube are in competition and complex spatial organization appears showing clusters of annular drop trains. In addition, the interaction between the flow in microtube and the imbibition in porous matrix leads to non-linear phenomena. In particular, decreasing the saturation in the porous matrix may slightly increase the flow rate in the microporosity for specific parameters. This non-linear analysis highlights the crucial role of wettability in the fluid transfer.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 421

Assessment of hydrogen uptake ability of clay-rich caprocks

Authors: Mohammad Masoudi[1]; Mohammad Nooraiepour[1]; Helge Hellevang[1]

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Underground Hydrogen Storage (UHS) has the potential to play an important role in the transition to renewable energy resources. In geological hydrogen storage, safety and efficiency are principal factors. We want to be able to get back as much as possible of the stored hydrogen and it is important that the seal can hold the injected hydrogen. One of possible leakage paths is through caprock. Hydrogen can migrate through the caprock within the pore solution. H2 molecules which are extremely small, can diffuse (or even advect) through pores and/or fractures of the seal. To do a throughout risk analysis, we need to assess the amount of hydrogen loss through caprock. Therefore, hydrogen transport properties in caprock in terms of uptake ability and diffusion are extremely important. However, due to the safety concerns of working with hydrogen gas (high diffusivity, low interaction energy, invisible flame, etc.) there is few data on the interaction of hydrogen gas with different natural settings. In this work we provide hydrogen uptake capacity of several natural materials (several Norwegian and international caprock samples). We used high-pressure gas adsorption analyzer to obtain the hydrogen sorption isotherms and hydrogen diffusion coefficient for the shale and clay samples. The data can be used for risk assessments of geological hydrogen storage in depleted hydrocarbon reservoirs and saline aquifers.

Participation:

In-Person

References:

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Poster / **422**

Modeling Two Phase Flow in Fractured Rocks Considering Hydromechanical Behaviour and Fluid Leakage

Authors: Zhen Zhang[None]; Xupeng He[None]; Yiteng Li[1]; Marwa AlSinan[2]; Hyung Kwak[3]; Hussein Hoteit[4]

[1] *King Abdullah University of Science and Technology*

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Introduction
Understanding the fundamental mechanism of the hydromechanical process and fluid leakage is crucial in modeling fractured reservoirs. Traditional simulation methods often assume impermeable and rigid fracture walls, which neglects the effects of fracture deformation and fluid leakage. This work introduces a Darcy-Brinkman-Stokes method to capture the effects of fracture deformation and fluid leakage in modeling the fluid flow in fractured rocks.

Methodology
To deal with the multiscale feature in fractured media, we employ the Navier-Stokes equation to model the fluid flow within the fractures and use Darcy's law to represent the flow with porous media. We then apply the stress-seepage model, based on Biot's poroelasticity theory and Terzaghi' s effective stress theory, to capture the geomechanical deformation. Specifically, we use the Darcy-Brinkman-Stokes method to achieve this goal, in which a unified equation is deployed to model the flow both in the fractures and the porous media. By tuning the range of the porosity and permeability, the Darcy-Brinkman-Stokes can mimic the Navier-Stokes equation within the fracture and Darcy's law within the porous media. We then conduct various sensitivity analyses to investigate the leakage effects by varying the fracture and matrix permeability, fracture roughness, effective normal and shear stress, and Reynolds number.

Results and Conclusions
The velocity and pressure profiles demonstrate the eddy area's exits, which significantly block the fluid leakage between the fracture and matrix. We also observe the apparent effects of the degree of the fracture roughness, effective normal and shear stress, and inertia on flow predictions in modeling the fluid flow within the fractures. The hydraulic properties can be significantly affected under high fracture roughness, high matrix permeability, high effective normal stress, and low Reynolds number condition. We then verify the observations in laboratory tests. The lab tests demonstrate that the

proposed method can predict the permeability well under different effective normal and shear stress, fracture roughness, inertia, and Reynolds number. Regarding the effective shear stress condition, the fracture aperture and permeability can be enhanced even with the increase of the effective normal stress. This situation could occur as long as more openness of the fracture caused by shear dilation exceeds the closure induced by the increase of effective normal stress.

We develop a fully coupled model to capture the hydromechanical behavior and fluid leakage in modelling two phase flow in fractured rocks. To our knowledge, the fully coupled framework is developed and applied to characterize fracture aperture displacement, further permeability change, and fluid leakage between fracture and matrix at the pore scale in fractured rocks for the first time.

Participation:

In-Person

References:

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MS10 / **423**

Attention-Res-UNet-based WGAN-GP Network to Boost Digital Rock Image Resolution

Authors: Xupeng He[None]; Yiteng Li[1]; Zhen Zhang[None]; Marwa AlSinan[2]; Hyung Kwak[3]; Hussein Hoteit[4]

[1] *King Abdullah University of Science and Technology*

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1. OBJECTIVE/SCOPE (25-75 words)
High-quality digital rock porous images are required hours to obtain using micro-Computed Tomography (⊠-CT), while low-quality digital rock images only take a few minutes. To reduce the scanning time while keeping the high-resolution pore structures, we propose an Attention-Res-UNet-based Wasserstein generative adversarial network with gradient penalty (WGAN-GP) to rapidly restore noisy ⊠-CT images to their clean counterparts.
2. METHODS, PROCEDURES, PROCESS (75-100 words)
There are mainly four steps within our workflow. Step 1: We extract numerous subsamples from the original rock image with data augmentation techniques to obtain sufficient training datasets. Step 2: train the Attention-Res-UNet-based WGAN-GP using the low-resolution rock porous images and the corresponding high-resolution rock porous images, in which the generator is composed of a Res-UNet with attention mechanism, and the loss in each layer is extracted to boost the predictivity, as shown in Figure 1. A VGG loss is combined to enhance the capability of capturing important features. Step 3: we conduct high-resolution Navier-Stokes simulations for the generated high-resolution images and the corresponding ground truth to calculate the permeability and relative permeability.

Step 4: We then compare the calculated physical properties and the difference maps between the generated images and the ground-truth images. If the physical properties are significantly different and the difference maps contain large errors, we need to check the accuracy of the Attention-Res-UNet-based WGAN-GP.

3. RESULTS, OBSERVATIONS, CONCLUSIONS (100-200 words)

Two datasets on 2D and 3D rock porous images demonstrate that the proposed Attention-Res-UNet-based WGAN-GP can successfully boost the resolution with minor errors. We further compare the performance of the proposed model with traditional Super-Resolution GAN (SRGAN) and Enhanced Super-Resolution GAN (EDSR). Our proposed method achieves the highest accuracy with the same dataset. The Attention-Res-UNet-based WGAN-GP outperforms other models because 1) the individual loss in each layer is combined with the final loss, which helps the network generate better feature representation at each layer; 2) the attention mechanism helps the network capture the most relevant features; 3) the residual block's utilization in Res-UNet alleviates the gradient vanishing problem and boosts information exchange across different layers; 4) the pre-trained VGG network helps the network to extract high-level features, and 5) the use of WGAN stabilizes the training process by surpassing the Jessen-Shannon divergence.

4. NOVEL/ADDITIVE INFORMATION (25-75 words) no more than three sentences

We propose a novel super-resolution approach using Attention-Res-UNet-based WGAN-GP to boost the resolution of 2D and 3D rock porous images, which is superior to the traditional models regarding accuracy and efficiency. This method enables us to obtain high-resolution rock porous images for real-time analysis.

Participation:

In-Person

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Poster / 424

Rock thermal properties prediction based on acoustic wave velocity in geothermal reservoirs

Author: Parvin Kolah Kaj[None]

Co-authors: Phil Vardon [1]; Hemmo Abels [1]; Auke Barnhoorn [1]

[1] *Delft University of Technology*

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Energy transition and the current ambition of the geothermal industry requires the exploitation of currently used sedimentary aquifers in adjacent sites and the exploration of new reservoirs in distant locations or deeper underground layers. In new areas, physical, mechanical and thermal properties of rock are needed for correct reservoir characterization and implementing a geothermal project safely and economically. The problem is that most of the available data come from hydrocarbon wells that are not necessarily in a favourable place for geothermal activities. Geothermal projects do not normally generate rich datasets and the lack of appropriate methodologies to convert downhole logs to rock properties slows down the increase in the number of geothermal doublets. Hence, it is

often impossible to predict rock properties with sufficient accuracy to evaluate geothermal project performance and reduce uncertainties in quantifying the risks of induced seismicity and drilling. In this study, we aim at predicting rock thermal properties including thermal conductivity, and thermal diffusivity based on wireline logs. Ultrasonic techniques are increasingly being used in various fields such as mining, geotechnical, civil and underground engineering. As they are non-destructive and easy to apply, they are employed both in situ and in the laboratory to characterize the dynamic properties of rocks.
Many studies have shown that the thermal conductivity of a porous rock depends mainly on the mineralogical composition, porosity of the rock, presence of fluids filling the pores, and ambient temperature and pressure. Porosity and thermal conductivity play an important role in the transport properties of fluid-rock interactions and the characterization of building materials. To inspect the relation between acoustics and rock thermal properties, rock samples from three wells in the North sea have been studied. Our results confirm the correlation between thermal conductivity and P-wave. In addition to P-wave, the travel time of S-wave through these sandstone samples has been recorded. The major difference between P and S waves is that due to their wave movement, P waves travel through any kind of material, whether it is a solid, liquid or gas. On the other hand, S waves only move through solids and are stopped by liquids and gases. For this reason, S waves are sometimes referred to as shear waves because they are unable to alter the volume of the material that they pass through. This also accounts why fewer S waves are recorded than P waves. The difference between P and S-waves could be representative of total void space within rock. The increase in Vp-Vs means the volume of non-solid part of the rock increases that is why shear wave cannot propagate through the samples as good as P wave.

Participation:

In-Person

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Poster / 425

Mixed-dimensional models for simulation of reactive transport in fractured porous media

Author: Shin Banshoya[None]

Co-authors: Eirik Keilegavlen [1]; Inga Berre [1]

[1] *University of Bergen*

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Numerical simulations of reactive transport in fractured porous media are necessary for several environmental and engineering applications. Networks of fractures may behave as shortcuts for the transport processes, whereas chemical reactions trigger mineral dissolution and precipitation that alter the porous medium and fracture walls locally. This will either cement flow paths or open new

ones, impacting the global flow regime.
In this talk, we present an approach to simulate reactive transport in fractured porous media, where dissolving and precipitating minerals might alter the flow characteristics. Our numerical solution strategy is based on a discrete fracture-matrix model with a mixed-dimensional representation of the fractured media. The model equations consist of coupled partial differential equations for the fluid flow, heat transfer and solute transport and non-linear algebraic equations representing the chemical reactions. The mineral dissolution and precipitation are formulated as a complementarity problem. The partial differential equations are discretized using finite-volume methods, and the resulting non-linear system of differential-algebraic equations is solved by Newton's method.
Numerical tests illustrate our model's ability to capture the tightly coupled physical and chemical processes and the two-way interaction with the fractures. Moreover, we discuss application of our framework to simulations representative of, e.g., geothermal field cases, where stability and computational cost become major concerns.

Participation:

In-Person

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MS10 / **427**

Flow field analysis towards improved predictability of diffusive flux in host rocks for radioactive waste

Authors: Cornelius Fischer[1]; Till Bollermann[1]; Johannes Kulenkampff[1]

[1] *Reactive Transport Department, Institute of Resource Ecology, Helmholtz-Zentrum Dresden Rossendorf (HZDR)*

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The predictive power of numerical approaches for the analysis of flow fields and, e.g., radionuclide migration, depends on the quality of the underlying pore network geometry. Validation of the obtained simulation results can only be performed with a limited number of methods. Positron emission tomography (PET) is a suitable technique that has been established in geomaterial sciences in recent years. The employment of appropriate radiotracers allows the analysis of advective transport and diffusive flux in a variety of complex porous materials.

In addition to the visualization of time-resolved transport patterns, the quantitative and statistical analysis of transport controlling parameters is currently in the focus of investigations using PET techniques. First, local transport properties can be extracted from single voxels or voxel layers of the flow tomograms. Second, the analysis of spatially correlated data sets, e.g. density data from micro-computed tomography (µCT) analyses, is the focus of interest. The purpose is to statistically compare the range of material heterogeneity with the range of transport heterogeneity and to derive generalizable conclusions.

Using low-permeability potential host rock types for underground radioactive waste repositories as examples, we analyzed the heterogeneity of the flow field at the laboratory scale 1. Reliable

predictions of diffusive flux heterogeneity are critical for assessing sealing capacity. We identified diagenetic and sedimentary subfacies components based on the concentration of diagenetic minerals and grain size variability, and quantified their pore size distributions and pore network geometries. The resulting generalized pore network geometries are used in digital rock models to calculate effective diffusivities, using a combined upscaling workflow for transport simulations [2]. Diffusion experiments analyzed with PET confirmed the simulation results and provided quantitative insights into the heterogeneity of diffusive flux. We introduced a statistical treatment of the PET and µCT tomographic datasets based on the spatial variability of both PET tracer concentrations and rock density. Targeting a generalized applicability, we present and discuss results on diffusive flux in different lithotypes. The focus of the comparison is on quantitative analysis of propagation heterogeneity and the correlation with data characterizing compositional homogeneity. Here we discuss possibilities of statistical evaluation of data from µCT analysis and their potential for correlation with PET analysis methods.

Participation:

In-Person

References:

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MS09 / 428

Pore scale study of freeze-drying using a non-isothermal pore network model and X-ray tomography image data

Authors: Nicole Vorhauer-Huget[1]; Maximilian Thomik[None]; Sebastian Gruber[None]; Petra Foerst[2]; Evangelos Tsotsas[None]

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Freeze-drying is investigated based on a non-isothermal pore network model of coupled heat and mass transfer 1. Simulations were carried out using image data from X-ray tomography (µ-CT) of freeze-dried maltodextrin, which was originally prepared with a solid content of c = 0.2 w/w solved in water [2]. Freeze-drying was conducted at a shelf temperature of -18℃ and a chamber pressure of 10 Pa [3]. The experimental parameters were used in the pore network simulation in which a domain size of 100x100x250 µm3 was considered. The pore network simulation provides data about the dynamics of the pore scale resolved sublimation front propagation as well as local temperature and pressure evolution and vapor diffusion rates. It can be shown and analyzed for

the first time how the sublimation front travels through the pore network in dependence of pore size distribution and various different process conditions. For this purpose, different temperature and pressure conditions were applied at the boundaries of the pore network. Besides µ-CT image data, also regular pore networks with different pore size distributions (monomal and bimodal) were implemented. The latter option is faster than imaging and image processing and allows to study more fundamentally different scenarios. This way, the evolution of the sublimation front can be studied at the limits of i) heat and ii) mass transfer controlled freeze-drying regimes as well as intermediate situations. As a result, the conditions for the formation of either flat or structured sublimation fronts can be provided. The outcome of this study can thus be used as a base for the prediction of material collapse.

Participation:

In-Person

References:

1 Surasani, V.; Metzger, T.; Tsotsas, E. (2010) Drying simulations of various 3D pore structures by a nonisothermal pore network model, Drying Technology 28 (5), 615-623
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[3] Foerst, P.; Melo de Carvalho, T.; Lechner, M.; Kovacevic, T.; Kim, S.; Kirse, C.; Briesen, H. (2019) Estimation of mass transfer rate and primary drying times during freeze-drying of frozen maltodextrin solutions based on x-ray -computed tomography measurements of pore size distributions, Journal of Food Engineering 260, 50–57.

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Energy Transition Focused Abstracts:

Poster / 429

Gradient hydrogel based on self-filtration

Authors: Clement de Loubens[1]; Hugues Bodiguel[1]

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Understanding and mastering gelation of biopolymer is important for controlling the structure of the gels and open the way to the design of micro-objects with a gradient of physical properties. In this study, we investigated the gelation between a calcium solution and a suspension of biopolymers. We showed that spontaneous osmotic flow through the gel controls its formation and can be used to a create concentration gradients.

For this purpose, we developed a quasi-bidimensional cell in which the suspension of aggregates at mass fractions below its gel point is brought into contact with a calcium solution. The diffusion

of calcium into the system allows the biopolymer to gel. We observed the propagation of the gelation front by microscopy. This front followed the classical diffusion-reaction laws, with a short-time regime limited by the reaction, and a long-time regime limited by the diffusion. We also used fluorescently labelled polymers to quantify the local concentration during the diffusion of calcium in the aggregate suspension.

Very surprisingly, the gelation mechanism induced a solvent flow from the biopolymer suspension to the calcium solution. This flow was characterized by the tracking of micrometric particles. A consequence of this flow was a local increase of the polymer concentration in the gelation front. We explain this phenomenon by the difference in chemical potential between the aggregates' suspension and the calcium solution. However, by analogy with osmotic phenomena in U-tubes, this implies that the forming gel acted as a semi-permeable membrane for calcium ions.

We illustrated the interest of his osmotic phenomenon to produce fibers based on protein fractal aggregates with a core-shell structure. The suspension of aggregates was co-injected with a solution of calcium chloride. Sol-gel transition of the suspension was induced by diffusion of calcium ions in the jet and ionic cross-linking of the proteins. The production of these fibers required a precise control of both hydrodynamic and physicochemical conditions, that were systematically investigated. Hydrodynamic instabilities competed with the gelation kinetics. Increasing the calcium concentration, several regimes were observed: swollen, dispersed, and shrunk fibers. In the first regime, homogeneous fibers were obtained. In the last one, osmotic phenomena led to a spontaneous core-shell structure with a dense shell.

Participation:

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MS10 / **430**

3D X-ray micro-velocimetry of unsteady multiphase flows in porous media

Authors: Tom Bultreys[1]; Sharon Ellman[2]; Christian M. Schlepütz[3]; Matthieu Boone[4]; Mostafa Borji[1]; Gulce Kalyoncu[None]; Niloofar Moazami Goudarzi[None]; Shan Wang[None]; Wannes Goethals[1]; Stefanie Van Offenwert[1]; Veerle Cnudde[1]

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Multiphase flow in porous media is an important process in a variety of Earth science applications, from groundwater remediation to subsurface CO2 and H2 storage. The associated pore-scale flow dynamics have been the subject of active research for decades, due to their non-linear nature and the difficulty of measuring and modeling them in the complex pore geometries of geo-materials. While progress in X-ray micro-computed tomography (micro-CT) has enabled to investigate the morphology of fluid distributions and menisci (Singh et al. 2019), measurements of the underlying flow dynamics (i.e. flow velocity fields) have remained impossible. This is because state-of-the-art micro-velocimetry techniques either require optically transparent porous samples with index-matched fluids, or do not currently provide the necessary spatial and temporal resolutions.
In this work, we present a breakthrough in 3D X-ray particle tracking velocimetry applied to capillary-dominated drainage in porous sintered glass and Ketton limestone samples. The method builds further on our lab-based X-ray velocimetry method (Bultreys et al. 2021), extending it to synchrotron micro-CT at the TOMCAT beamline of the Swiss Light Source. Time resolved tomography at 250 ms per tomogram and 2.75 µm voxel size was used to track µm-scale tracer particles in the non-wetting phase while it was injected into the pore space at a constant low flow rate. Our results showed that Haines jumps caused fluctuations in the flow field of the non-wetting phase, with local velocities exceeding the interstitial (injection) flow rate by up to two orders of magnitude. In accordance with previous studies based on, e.g., pressure measurements, the main fluid displacement during Haines jumps took place on the order of 1 to a few seconds. Subsequently, the resulting velocity fluctuations decayed over tens of seconds. Contrary to prior studies, our results also give insight into the spatial structure of the fluctuations. The velocity fluctuations originating from Haines jumps propagated through the porous medium as rolling waves with speeds on the order of mm/s - much slower than the speed of pressure waves (i.e., the speed of sound in the non-wetting phase, ~km/s) –accompanied by retraction of fluid menisci in locations away from the main Haines jump. Such velocity waves reached long distances into the porous medium, with decay lengths exceeding 30 times the characteristic pore size, where the velocity magnitude was still an order of magnitude higher than the injection rate. This indicates the possibility for long-range non-local effects due to capillary instabilities during drainage. Successive Haines jumps reactivated flow paths in the same regions, which appeared to have similar decay times.
The results presented here are the first pore-scale velocimetry measurements of (unsteady) multiphase flow in rocks and possibly in any 3D porous material. The study sheds light on the spatial and temporal structure of capillary fluctuations in 3D porous media, which are of central importance in newly emerging upscaling theories for multiphase flow (McClure et al. 2021).

Participation:

In-Person

References:

Bultreys, T., van Offenwert, S., Goethals, W., Boone, M. N., Aelterman, J., & Cnudde, V. (2022). X-ray tomographic micro-particle velocimetry in porous media. Physics of Fluids, 34(4), 042008. https://doi.org/10.1063/5.0088000

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Energy Transition Focused Abstracts:

MS13 / 431

Nanometer-scale wetting of micro- and meso-porous carbons: a time-resolved synchrotron small-angle scattering analysis

Author: François Chaltin[1]

Co-authors: Mouna Hamid [2]; Bart Goderis [2]; Cédric Gommes [1]

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Many applications of nanoporous materials require their porosity to be filled with liquid. This is notably the case in heterogenous catalysis or in electrochemistry. In all cases, it is essential to determine whether the porosity is uniformly filled or whether the liquid is excluded from specific pores. In a macroscopic context, wetting is well predicted in terms of the different energies of the wet and dry surfaces. By contrast, the conditions for wetting of nanoporous solids are still poorly understood. It is unclear whether or not macroscopic physical concepts apply at scales close to molecular dimensions. Moreover, the geometry of porous media can be complex with pores with a variety of sizes and connectivity. Besides the spontaneity of the pore space liquid invasion, other important questions concern the kinetics of the problem in relation with the permeability of the different pores, which makes the question even more challenging.

In the present study, we investigate the nanometer-scale wetting of nanoporous materials. Specifically, we focus on carbon xerogels with two families of pores, namely, mesopores with sizes around 20 nm coexisting with micropores having almost molecular dimensions. We perform capillary-rise experiments of water in these materials, and we use synchrotron Small Angle X-ray Scattering (SAXS) to investigate the process at nanometer scale in a space- and time-resolved way. Different materials are considered with different meso- and micro-porous structures. We also report capillary-rise experiments on materials with water-saturated micropores by preliminary adsorption of water vapour. All experiments were performed at the Belgian DUBBLE station (BM26) at the European Synchrotron Radiation Facility.

Our results reveal a two-stage wetting process, with a diffuse water front coming first, followed by a sharp front lagging a few millimetres behind. The SAXS data shows that the diffuse front corresponds to the early filling of the molecular-sized micropores, while the sharp front corresponds to the later filling of the mesopores. The two water fronts propagate according to a $\sqrt{t}$ law, which is typical of a Washburn model whereby the wetting kinetics is limited by viscous dissipation. We use independent water adsorption experiments to estimate the capillary suction into the micropores, from which we infer their permeability.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS01 / **432**

Properties of restructuring porous media for thermochemical energy storage

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Co-authors: Torben Prill [1]; Thomas Jahnke [1]; Marc Linder [1]

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A significant part of the overall energy consumption is related to the provision of heat –for heating of buildings and tap water as well as for industrial processes (e.g. around 54% for Germany in 2010-2020 1). Considering this as well as the fact that this thermal energy is still mainly provided using fossil fuels (above 70% for Germany in 2020 1), energy transition is also a transition of the heat supply.
One challenge concerning this heat transition is the storage of thermal energy. Depending on the application and energy source, targeted storage times can be over short (hours) as well as long periods (seasonal). Additionally, thermal energy can be stored and used directly, or conversion to and/or from a different energy form is involved (e.g. power-to-heat).
A highly promising way to store thermal energy is by converting it to chemical energy using reversible gas-solid reactions. The energy stored as chemical potential utilizing the endothermal decomposition of a solid to a solid and a gas can be recovered at any chosen time –minutes or years after the storage process –as long as the components are kept apart from each other and any other potential reaction partners. To recover the stored energy, gas and solid are recombined and the exothermal formation of the initial solid compound takes place, releasing the stored thermal energy. Depending on the chosen reaction system, a wide range of storage temperatures can be covered (sub-zero [2] to above 1000 ℃ [3]).
Due to the necessity of a high accessible surface area of the solid reaction partner, these storage materials are porous media mainly consisting of (consolidated) granular matter. According to the thermodynamic equilibrium of such reactions, solid temperature and reaction gas pressure are dependent on each other: The higher the reaction gas pressure, the higher the equilibrium temperature. It is therefore imperative for the application of the materials in thermochemical energy storage to evaluate solid properties such as thermal conductivity and permeability to the reaction gas. However, as the storage process involves the transformation of one solid to another, these properties change significantly as the solid structure is changing.
Our contribution aims to improve the understanding of the impact of the structural changes of thermochemical storage materials on the transport properties of the porous medium. Based on experimental results on reactor as well as particle scale, we discuss the evolution of the solid structure with a focus on the effects on the reaction behaviour.

Participation:

In-Person

References:

1 Report of AG Energiebilanzen e.V., Anwendungsbilanzen zur Energiebilanz Deutschland, May 2022
[2] Muthukumar, P. and Groll, M., Metal hydride based heating and cooling systems: A review, International Journal of Hydrogen Energy 35(8) (2010) 3817-3831.
[3] André, L. et al., Screening of thermochemical systems based on solid-gas reversible reactions for high temperature solar thermal energy storage, Renewable and Sustainable Energy Reviews 64 (2016) 703-715.

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MS10 / **433**

3D Pore Roughness Extraction Technique: From 1.0 (2D) to 2.0 (3D)

Authors: Yiteng Li[1]; Xupeng He[None]; Zhen Zhang[1]; Marwa AlSinan[2]; Hyung Kwak[3]; Hussein Hoteit[4]

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OBJECTIVE/SCOPE
Surface roughness is a sneaky troublemaker for interpreting pore size distribution from NMR T2 responses. Thus, it is of vital importance to characterize surface roughness and quantify its effect on NMR T2 relaxation. In our preceding work, the 3D pore roughness was evaluated by weighted averaging of the roughness measurements of 2D thin sections. This work presents a new-generation pore roughness extraction technique for real 3D surface roughness measurement.

METHODS, PROCEDURES, PROCESS
This work aims to develop a novel image-based roughness extraction method measuring surface roughness from a 3D benchmarking surface. The proposed workflow has four main steps, including the voxel surface diagnosis, smooth surface reconstruction, benchmarking surface generation, and 3D roughness parameterization. The first step is to examine if any vacancies or discontinuities exist on the voxel surface. A topology fix operation will be applied if necessary. Then we use the spherical harmonic method to reconstruct the smooth surface and the benchmarking surface with the volume conservation constraint. Height variations between two surfaces are evaluated, as a metric of surface roughness, and then converted to a 3D surface plot for roughness parameterization. We characterize the surface roughness using the pore roughness coefficient (PRC), defined in our previous work, and a 3D PRC value will be evaluated for each pore structure.

RESULTS, OBSERVATIONS, CONCLUSIONS
The accuracy of the proposed method is first validated with regular pore shapes (e.g. spherical, cube, tetrahedron) with smooth surfaces. As expected, the surface plots exhibit horizontal planes across 0, implying the proposed method can handle any pore shape even free of roughness. Then we measure the surface roughness of synthetic rough pores designed in our previous work, and compare 3D PRC values with the previous ones. Numerical results demonstrate another expectation that 2D image thin sections may not fully capture the roughness heterogeneity and anisotropy in the 3D space. It is worth noting that the key to the success of roughness measurement is the determination of the benchmarking surface from which the surface height variations are calculated. When creating the benchmarking surface, it is necessary to examine if the created surface excludes the fine-scale textures as much as possible and meanwhile the volume enclosed by the surface remains the same. In the end, the proposed method is applied to measure the surface roughness of real pore structures; a physically meaningful T2 correction factor is derived as a function of roughness intensity.

NOVEL/ADDITIVE INFORMATION
We improve our image-based pore roughness extraction method to measure surface roughness directly from 3D benchmarking surfaces. The proposed method is robust, regardless of pore shape, surface roughness heterogeneity, and anisotropy. Thus, this work offers an accurate and effective approach to characterizing the surface roughness of pixelated porous structures.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 434

Semi-Analytical Model to Predict Dynamic Capillary Pressure - Water Saturation Relationships for Multiphase Flows in Porous-Media

Authors: Harris Rabbani[1]; Saideep Pavuluri[1]

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The capillary pressure defines the difference in pressure between the non-wetting and wetting fluids. The capillary pressure is part of the flow governing equations and its definition can have a profound impact on the nature of fluids displacement in a multiphase flow environment. Conventionally, the capillary pressure - saturation relationships are determined under equilibrium conditions which signify that all the fluid-fluid interfaces that exist at the pore-scale maintain a static configuration at a certain instant in time. However, there exist experimental and numerical evidences that state that the dynamic nature of fluid flows indeed play a prominent role in defining the trends of the capillary pressure - saturation relationships. In this work we develop a first of a kind semianalytical model to predict the capillary pressure - water saturation curves during piston-like drainage displacement by integrating the dynamics of fluid flow based on fundamental laws of fluid mechanics.

The proposed semi-analytical model can potentially be incorporated into existing multiphase flow simulators to rapidly compute the capillary pressure at various saturations of the flow medium under dynamic flow conditions. The presented semi-analytical model has been validated against experimental and numerical data sets available in literature at various flow conditions and considering different sets of fluid properties. We noticed a satisfactory match of the results predicted by the proposed semi-analytical model against the literature data. After performing a holistic sensitivity analysis, we notice that the properties of the porous medium, fluids and the fluid-solid interactions play a significant role in defining the trends of the capillary pressure - saturation curves.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS03 / **435**

New algorithms for numerical simulation of multiple hydraulic fractures in low permeability rocks

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Modelling of multiple fractures in hydraulic fracturing is of importance for creating a complex fracture network and enhancing the productivity of resources in underground reservoirs. In this work, multiple hydraulic fracturing in low permeability media is studied by extended finite element method (XFEM) and the governing equations for fluid flow and elastic rock are introduced. Two robust algorithms are presented to couple the two media (rock and fracturing fluid) for discretized model in plane strain condition. The algorithms include: 1) stress transfer from fluid to rock matrix and 2) evolution of fracture opening width, resulting in the change of fluid pressure. An iterative process is demonstrated for the interaction of the two media to promote convergence. The coupled model for multiple hydraulic fracturing is developed to express the interaction between the model parameters, combined with the process of fracture propagation. To verify the results, the shadow effect between fractures is analysed by showing the stress change alongside the propagating fractures.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 436

Effect of CO2 dissolution on elastic instabilities of the polymer through porous media

Authors: Mohsen Mirzaie Yegane[1]; Esther Zijlstra[2]; Ali Fadili[3]; Diederik van Batenburg[4]; Thierry Leblanc[5]; Pouyan E. Boukany[6]; Pacelli Zitha[2]

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CO2 flow in porous media often results in poor reservoir sweep efficiency. To mitigate this problem alternate injection of a polymer solution and CO2, known as Polymer-assisted Water-Alternating-Gas (PA-WAG), is applied. The objective of PA-WAG is to improve mobility control, thus sweeping a larger part of the reservoir. Therefore, it is of great importance to study the effect of CO2 and polymer interaction to address the feasibility of PA-WAG.
The objective of this study was to investigate the impact of CO2 dissolution on (a) physical polymer properties (e.g., viscosity and pH), and (b) elastic instabilities of polymer flow in porous media. The following experiments were performed. Firstly, an ATBS-based polymer (SAV 10) solution was prepared in synthetic seawater in an oxygen-free environment. The polymer solution was afterward saturated with CO2 at the reservoir conditions (i.e., T=40 degrees Celsius and P=20 bar) and then it was forced through a capillary while maintaining the same temperature and pressure. Consequently, the apparent viscosity and pH were recorded in real time over the course of 29 days. The CO2 molar concentration in the polymer solution was around 0.3 mol/L which was the solubility limit of CO2 in water at the reservoir conditions. Secondly, the polymer solution with and without the dissolved CO2 was injected into a microfluidic system of periodic arrays of circular pillars in a staggered layout at negligible inertial effect. Apparent viscosity was measured at various shear rates (or Weissenberg numbers). Moreover, the instabilities of polymer flow through porous media were visualized using an inverted fluorescence microscope connected to a high-speed camera.
As a result of the flow of CO2-saturated polymer into the capillary, the viscosity dropped to around 53.5 of its initial value after one day but recovered some of it, and after 29 days, the polymer maintained around 83.5 of its initial viscosity. The initial decrease was due to the formation of carbonic acid and neutralization of the charges on the polymer backbone leading to a decrease in both pH and viscosity. The recovery of viscosity was because of the evolution of the ammonium ion due to the hydrolysis of the amide groups resulting in an increase in pH as well as viscosity. Moreover, the CO2 dissolution had the following impacts on the viscoelasticity of the polymer: (a) under a rheometer, it delayed the onset of shear-thinning from 4.2 1/s to 10.0 1/s (b) in the microfluidic, it also delayed the onset of shear-thickening from 15.5 1/s to 20.5 1/s. Elastic flow instabilities beyond the onset of shear-thickening were evident from visualization of the flow streamlines. We present the mechanism of the elastic instability and characterize it based on strong temporal fluctuations in pressure drop.

Participation:

In-Person

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Poster / 437

Further Analysis of the Flow through Porous Bodies with Application to Stormwater Management

Author: Ana Barcot[1]

Co-authors: Sofia Larsson [1]; Hans Åkerstedt [1]; Staffan Lundström [1]

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In the work of Lundström et al 1, a new concept of stormwater storage in sponge-like porous bodies (SPBs) is suggested: down-flow and up-flow SPB storage. The analytical and numerical results of the analysis based on the first principles argue that the studied up-flow model can capture and control the stormwater runoff for various conditions of Swedish design rainfalls. In the present research study additional work on the existing model is carried out.

The model presented 1 consists of a solid cylinder (radius δ) surrounded by an inner and outer porous annulus (radii a and b respectively, where b>a). The inner and outer porous media is made of thin vertical cylindrical fiber rods with dimensions Ri,Ro « a, b, δ, where Ri and Ro represent their respective radii. For such a model of the water uptake, the governing equation is the Darcy Law, and the flow is mainly driven by the capillary action ($\Delta p \propto 1/R$). Further advances of the model are presented in this research including the diffusion of water into the dry soil, for which the diffuse-front modeling, as done by Zarandi and Pillai [2] (Richard's equation), is applied. The corresponding set of equations for the motion of liquid fronts for each of the channels with the corresponding boundary conditions are given and the pressure quantities are averaged over the cross-section. Numerical integration is carried out in MATLAB. The diffuse-front model is resolved with COMSOL Software using Porous Media Flow Module. The numerical simulation results will be validated against the experimental measurements planned on a physical up-flow model in the laboratory setting. Similarly, to the work of Lundström et al 1, the model storage inflow rates and volume absorption will be plotted against time and compared to the Swedish design rainfall data.

References:
1 Lundström, T. Staffan, et al. "Dynamic distributed storage of stormwater in sponge-like porous bodies: Modelling water uptake." Water 12.8 (2020): 2080.
[2] Zarandi, Amin, and Krishna M. Pillai. "Application of Sharp-and Diffuse-Front Models for Predicting Mass Gain and Saturation in Fibrous Wicks." (2018).

Participation:

In-Person

References:

1 - Lundström, T. Staffan, et al. "Dynamic distributed storage of stormwater in sponge-like porous bodies: Modelling water uptake." Water 12.8 (2020): 2080.

[2] - Zarandi, Amin, and Krishna M. Pillai. "Application of Sharp-and Diffuse-Front Models for Predicting Mass Gain and Saturation in Fibrous Wicks." (2018).

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Poster / **439**

Impact of Relative Permeability Hysteresis in Numerical Simulations of Underground Hydrogen Storage in Porous Formations

Authors: Guillermo Giacomi[1]; Luis Cueto-Felgueroso[2]; Marco Dentz[3]

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Renewable energy sources have a significant disadvantage as building blocks of a decarbonized energy system: they rely heavily on weather conditions, which can cause fluctuations in energy generation. To address this issue, hydrogen (H2) is increasingly being seen as a viable way to transport excess energy generated by renewable sources, preventing imbalances in energy supply. However, storing H2 is a challenge due to its low volumetric energy density, which requires large storage sites. Underground porous media, such as confined aquifers and depleted hydrocarbon reservoirs, seem to be the most feasible option for H2 storage.

Enabling the large-scale implementation of underground storage of hydrogen requires a multidisciplinary effort, including the study of multiphase flow processes during the injection of H2 into underground porous media. Our main goal is to numerically investigate how the displacement of brine by hydrogen affects recovered gas purity, and losses due to hydrogen dissolution and residual trapping.

We focus on the processes of capillary trapping and spatial heterogeneities in the hydraulic properties of the medium. To evaluate the spreading of the saturation front due to spatial heterogeneities, we model the immiscible displacement of brine by hydrogen. Understanding front spreading due to viscous and gravitational instabilities is important because spreading can enhance hydrogen dissolution and entrapment. We simulate multiple cycles of H2 injection/production over a test volume, incorporating hysteresis in the relative permeability to study how this condition impacts hydrogen dissolution, purity, and recoverability. We compare cases with and without hysteresis to investigate the role of viscous forces and heterogeneity alone. These cycles also help us understand the balance between fingering stability and gravity override. Finally, we perform a dynamic reservoir simulation on a more realistic reservoir geometry, taking into consideration the elements already discussed.

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Poster / 440

Mechanisms of Solute Mixing in Darcy's scale Heterogeneous Formations

Authors: Aronne Dell'Oca[1]; Marco Dentz[1]

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Solute mixing in porous media plays a fundamental role in a variety of contexts, e.g., environmental risk assessment, geochemical reactive transport. Mixing dynamics are strongly impacted by the heterogeneity of the hosting porous media which leads to inhomogeneity of concentration within the spreading and the mixing volume. Considering Darcy's scale heterogeneous formations, we develop a randomly dispersive lamellae approach in which the variability in the dispersion rates of the lamellae that constitute a solute plume is recognized as a fundamental aspect of the mixing dynamics. The framework allows rending the inhomogeneity of the concentration distribution within the mixing volume before the late time well-mixed condition is reached. Furthermore, In light of the hidden (data scarcity) and heterogeneous nature of environmental porous formations, the degree of mixing of a solute plume is uncertain. The proposed randomly dispersive lamellae framework represents a strategy to quantify the latter. We test our approach for mildly to highly heterogeneous formations.

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MS10 / 442

Spatio-temporally Resolved Dynamical Transitions in Flow of Pickering Emulsions through Porous Media

Authors: Milana Trifkovic[None]; Steven Bryant[None]; Aigerim Meimanova[None]; Leonardo Martin-Alarcon[None]; Guofeng Yang[None]; Brandy Kinkead[None]; Aleksandra Govedarica[None]

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Imaging fluid flows provides valuable physical insight, especially for complex fluids as emulsions, foams and dispersions. Unfortunately, high temporal and spatial resolution of flow in porous media still poses a grand challenge. In this study, we present a multiscale approach to study the spatio-temporal flow dynamics in realistic porous media of Pickering emulsions stabilized using attractive desulfated cellulose nanocrystal nanoparticles.

We take advantage of the rapid scan rate of a laser scanning confocal microscopy (LSCM) to capture flow through 3D granular porous media at high spatial and temporal resolution. We show that steady flow of such emulsions exhibits large-amplitude oscillations in pressure gradient which cannot be explained by geometric straining models, filtration models, or continuum rheological models. Using a custom-built micro-sandpack apparatus coupled with confocal microscopy, we present measurements that reveal localized spatio-temporal flow patterns of emulsions characterized by: particle attachment and deposition to nearby grains, droplet deposition, jamming of droplets within the throat, and release. The deposition/jamming/release is cyclical and corresponds precisely to the gradual-then-rapid changes in pressure gradient. The relative influence of particle loading on reducing the overall permeability of porous media and pressure gradient signature was evident. With higher particle loadings, the existence of nanoparticle deposits leads to more effective reduction of relative permeability of porous media and substantially higher pressures gradients were required to release the emulsion plugs.

Photonic force microscopy confirms the strength of droplet-droplet attraction and also reveals a new phenomenon, the formation of chains of nanoparticles which tether droplets together. The chains preserve strong attraction between droplets at nonzero separation distance and are likely to contribute to the persistence of droplet attachment to grains and of droplets deposited on droplets, which facilitates jamming.

These observations contribute to a growing body of evidence indicating complex spatiotemporal dynamics of Pickering emulsion flow through porous media, which cannot be described by the existing models. Flow of emulsions through porous media is important across a spectrum of scientific fields and applications including drug delivery, agriculture, oil and gas, and water treatment. With an initial application of a powerful multiscale approach, we provide measurements of evolving emulsion microstructure, local droplet velocity, precise measurement of droplet-droplet interaction, and lay a foundation to answer open questions about Pickering emulsion flow through porous media.

Participation:

In-Person

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MS02 / 443

Multiscale porous media approach to simulate shadowing and transpirative cooling effect of urban vegetation

Authors: Aytaç Kubilay[1]; Yongling Zhao[1]; Léopold Giroux-Gauthier[2]; Dominique Derome[3]; Jan Carmeliet[4]

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Vegetation like trees and grass is known to have a cooling effect that naturally enhances the thermal comfort for pedestrians in cities. While shadowing and transpiration by vegetation cool the urban environment during daytime, the blocking of cooling to sky by longwave radiation during night and increase in relative humidity might have an adverse effect. Also, while urban wind cooled by trees may have a cooling effect at downwind urban places lacking vegetation, dense trees may decrease the heat removal by ventilation from streets due to wind blocking effect. To study these complex interactions, a detailed vegetation model is needed to take into account the momentum, heat and moisture transfer processes taking place at different scales.

The authors developed over the years an urban microclimate model, coupling (1) a computational fluid dynamics (CFD) model for air, heat and moisture flow in the air domain, (2) a longwave and shortwave radiation model for radiative exchange between urban surfaces, sun and sky, (3) a coupled heat and moisture transport model for moisture transport in building facades, soil, pavements, and (4) a wind driven rain model. The set of equations is solved in OpenFOAM and the model is open source (urbanMicroclimateFoam at the Chair of Building Physics). Vegetation is modelled as a porous medium by introducing sink and source terms in the momentum, heat and moisture transport equations. The momentum sink is modelled by introducing a drag coefficient that depends on leaf area density. The heat and moisture transport from leaves is modelled by a leaf model depending on leaf area density in each vegetation cell, and the model accounts for convective and latent heat, and vapor transport depending on stomatal resistance. Solar radiation shadowing is modelled using a radiation attenuation model, while longwave radiation is modelled using a view factor method. Special shapes for trees based on Lidar information are introduced, limiting element discretization and taking into account the growth of trees. A special interface model is introduced for the modelling of heat and moisture exchange between grass, air and soil.

The model has been validated and applied to different case studies. In a first case study we analyze the influence of tree size on the pedestrian thermal comfort in street canyons. An optimal tree age of around 20-30 years is found, maximizing shadowing and transpirative cooling, while not blocking heat removal by air flow. A second example shows that, depending on wind direction, trees can cool down city parts down-windward, even when no trees are present at these locations. A third example shows the redevelopment of parking spaces as green areas on St. Helene island in Montreal and the possible cooling effects during heatwaves.

Participation:

In-Person

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Poster / 444

Simultaneous Interpretation Of Multiphase Fluid Flow Characteristics In Porous Media from Steady State SCAL Experiments Performed in a Microfluidic Approach

Authors: Bettina Jenei[1]; Hanin Samara[2]; Nils Langanke[1]; Roman Manasipov[3]; Safa Al-Ismaili[1]

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Introduction: This work aims to conduct, interpret and derive the multi-phase fluid flow behaviour more efficiently and feasibly from microfluidic experiments. The goal is to conduct SCAL experiments using a microfluidic setup on a chip. Additionally, interpret the in-situ results, where the parameters influencing the multi-phase fluid flow in porous media, such as wettability, capillary pressure, and relative permeability, are measured simultaneously. There are numerous economic and technical advantages of this approach. Conventionally, SCAL measurements are conducted through core samples using X-ray and multi-phase fluid flow parameters in porous media are measured separately. These properties can be simultaneously determined in digital rock physics (DRP) by applying micro-CT imaging but with high costs.
Materials and Methods: The steady-state method was utilised in this study and re-designed for microfluidic flooding. The measurement was conducted using one oleic and one aqueous phase, applying different fractional flow steps, mimicking the range of varying water saturation in the reservoir during the depletion process (imbibition). The used microchip has a synthetic pore-structure design with circular grain shapes. The measurements conducted are visible in real-time using a microfluidic approach.
Results: The experimental results show that it is possible to adapt the microfluidic flooding for conducting and interpreting SCAL measurements. An additional advantage of this method is that the wettability and capillary pressure could be successfully determined by means of image processing using only the data obtained from the steady-state method in a microchip. Since the measurements are visible live, and images of the microchip are captured with the desired frequency, the image processing facilitates the understanding and interpretation of multi-phase fluid flow in porous structures, which is not possible with cores. Overall, to overcome the technical and economic limitations of digital rock physics, the application of SCAL through microchips representing the porous media is a good alternative.
Addition: The SCAL-on-Chip is a promising approach to contribute in describing and analysing multi-phase fluid flow on a Darcy- and pore-scale. Image processing contributes to developing more feasible interpretation tools for estimating wettability and capillary pressure. It provides the possibility to derive mathematical models of the relationship between multi-phase flow characteristics. The derivation of a general function between the measured properties could be possible with machine learning and a sufficient amount of experiments using pore structures that closely resemble porous media.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS11 / 445

Impact of nanoparticles and gas composition on bubble density and coarsening rate of confined CO2-foam under high-pressure high-temperature conditions

Author: Aurora Pérez-Gramatges[1]

Co-authors: Juliana Maria da Fonseca Façanha [2]; Leandro Freitas Lopes [1]; Grigori Chapiro [3]; RODRIGO Weber dos SANTOS [4]; Felipe Ribeiro [1]; Pablo Godoy [1]; Luis Maqueira [1]; Giulia Fritis [4]

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The use of foam technology is a potential solution to control gas mobility in highly heterogeneous reservoirs. However, achieving stable CO2-foams under reservoir conditions can be challenging since the high solubility in water of supercritical CO2 enhances coarsening and coalescence of confined bubbles. Coarsening is characterized by the evolution of foam structure due to gas diffusion between bubbles, changing the average bubble size and foam texture. When foam texture coarsens, gas mobility control is impaired, and it can also affect foam rheology (Nonnekes et al., 2015). While most studies have focused on the dynamics of foam texture, which results from the balance between foam generation and destruction, few works have tried to evaluate foam coarsening for confined foams. In this presentation we will show the main results from a micromodel experiment where CO2-foam coarsening was reduced by using nanoparticles and/or a CO2/N2 gas mixture. A zwitterionic surfactant was used as base foaming agent, and different foams containing CO2 were injected into a micromodel at high pressure (10.3 MPa) and high temperature (60 ℃). Pressure drop, foam texture (bubble density), bubble growth regime, and flow characteristic were quantitatively assessed and related to gas mobility reduction obtained by gas trapping during the co-injection of gas and foaming fluids at 50% foam quality. Image analysis was performed without stopping the foam experiment or using a dye for image analysis, and used to calculate bubble density and size distribution of the foam confined in dead-end pores areas of the micromodel. The results showed that the CO2-foam stabilized only by surfactant showed poor behavior in porous media, while an improvement in both foam texture (bubble density at the inlet of the micromodel) and gas trapping was obtained using the nanofluid (Lopes et al., 2021). A larger decrease in gas mobility was obtained with CO2/N2 gas mixture, achieving the highest increase in pressure drop, which was attributed to the large number of trapped bubbles (2x higher than with nanofluid). This result suggested that using a gas mixture would be suitable to control gas mobility in high-permeability channels and to block thief zones. The coarsening rates (change in trapped bubble area with time) were reduced in both cases, indicating that the initial foam texture determined the resistance to flow (Façanha et al., 2022). The attempt to combine both strategies for reducing coarsening showed that nanoparticles decreased the pressure drop of the foam generated with the N2/CO2 mixture. Hence, injectivity concerns that might arise when injecting a gas mixture with a surfactant solution could be overcome by adding nanoparticles to the aqueous phase. The results of this work suggest that a minimum pressure gradient for strong foam generation can be achieved by simply tackling the foam destruction mechanisms rather than

changing injection conditions, showing the complexity of foam injection projects. Therefore, investigating the mechanisms of foam destruction at pore scale is fundamental for tailoring CO2-foam properties for field applications.

Participation:

In-Person

References:

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MS06-B / **446**

Impact of CO2 concentration in gas phase on foam behavior in carbonate rocks

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Foam-assisted water alternate gas injection (FAWAG injection) could be a promising technology to assist gas mobility control, consequently gas management in surface facilities of ultra-deepwater fields in the Brazilian offshore (Vieira et al., 2020). In these fields carbon dioxide (CO2) concentration in the gas stream varies, which can negatively impact foam stability, accelerating its destruction (Abdelaal et al., 2020). However, the impact of CO2 concentration in the gas stream is seldomly evaluated. In this work, we evaluate the impact of CO2 concentration in the gas phase on foam generation and foam strength (apparent viscosity) in porous media.

To this end, we conducted coreflood experiments where gas phase and surfactant solution were co-injected through Indiana limestone under relevant conditions (temperature –65□C, pressure –10 MPa and superficial velocity –3.5 x 10-6 m s-1). Four different gas compositions were used for the tests, namely nitrogen (N2), CO2 and two CO2-N2 mixtures (10 mol%, 50 mol%). Two commercial zwitterionic surfactants (CAHS –cocamidopropyl hydroxysultaine and CB –cetyl betaine) were used at 0.5 wt.% concentration (active matter) as foaming agents. The experiments were carried out with the core mounted in vertical position and the injection direction was bottom-to-top.

Our results have shown that increase in CO2 concentration in the gas phase decreased overall apparent viscosity (□foam), but no linear correlation has been found. Maximum □foam values for CB

ranging from 30 mPa s-1 for CO2-foam to 170 mPa s-1 for N2-foam. For CAHS, maximum foam values ranged between 70 mPa s-1 and 170 mPa s 1 for the same conditions. Gas composition also impacted transition foam quality (fg*), however, the changes in foam behavior as a function of gas fraction seemed to be dependent of the structure of zwitterionic surfactant. For CB surfactant, increased CO¬2 concentration in gas phase (10 mol% and 50 mol% CO2-N2) shifted foam transition quality to the lower gas fractions (from 0.6 to 0.4), indicating that coalescence was favored under these conditions. The apparent viscosity of the foam formed between CO2 and CB surfactant solution did not present a clear transition, and it remained constant as a function of foam quality. Under the same conditions, fg* for CAHS was shifted to the right (0.5 to 0.7), indicating that resistance to coalescence increased as a function of CO2 concentration on the gas phase for this surfactant. Another important observation was that from a gas fraction of 0.9, foam apparent viscosity was independent of gas composition. That meant that N2-, gas mixture- or CO2-foam had the same foam apparent viscosity (CAHS ~ 20 mPa s-1, CB ~ 10 mPa s-1), indicating that this regime was dominated by limiting capillary pressure. These findings suggest that for FAWAG project gas stream has considerable variation in CO2 concentration, the surfactant chosen not only needs to tolerate salinity and temperature of the reservoir, but also needs to maintain a high fg* under these changing gas composition conditions.

Participation:

In-Person

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Poster / 448

NMR relaxometry characterization of water adsorption in corn stover anatomical fractions

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Despite being major contributors to global CO_2 emissions, fossil feedstocks are finite natural resources frequently used to produce high value goods including fuels and plastics. One alternative is to replace fossil feedstocks with renewable agricultural feedstocks due to their ability to sequester carbon during growth. While a promising alternative, the use of food crops as feedstocks brings its own set of challenges. Recent emphasis has been placed on deconstruction of agricultural residues, such as corn stover, into fuels and chemicals. Polysaccharides from lignocellulosic plant cell walls can be converted to glucose, but biomass recalcitrance to enzymatic hydrolysis presents a practical challenge to this pathway. Pretreatment steps help improve enzymatic access to plant cell walls and once optimized, allow for these processes to be scaled. Nuclear magnetic resonance (NMR) relaxometry is applied to corn stover to gain a better understanding of these systems and the impacts of pretreatment. These measurements directly measure water adsorption in anatomical fractions of corn stover. NMR transverse T_2 relaxation time distribution measurements indicate multiple water populations, which vary with anatomical fraction and water adsorption. Measured T_2 data are used to calculate thermodynamic properties of Brunauer-Emmet-Teller (BET) adsorption theory using a model to estimate mono and bilayer relaxation. T_2 data are used directly to determine rotational diffusion correlation times indicating adsorption interaction strength. T_1-T_2 longitudinal-transverse relaxation time correlation measurements quantify differences in the molecular level structural order of the adsorbate surface water as a function of water activity, i.e. relative humidity or water vapor partial pressure. The T_1/T_2 ratio provides a measure of the surface energy related to the adsorption strength and surface diffusive mobility of the water adsorbate, and differentiates the anatomical fractions. The results indicate that direct measurement of NMR relaxation times can be used to characterize corn stover biomass water adsorption, which are data relevant to biomass processing and handling. These procedures may be extended to pretreated lignocellulosic materials to study how morphological changes impact adsorption, and applied to monitor enzymatic hydrolysis progress *in situ*.

Figure 1. Corn Stalk MRI. A 1 mm thick transverse slice taken of a hydrated corn stalk with a 25x25 mm field of view over 128x128 pixels for a resolution of 195 μm/pixel.

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Poster / 449

Potential Applications of Quantum Computing in Pore Scale Modeling

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The three major concerns of today's society that relates to the energy sector are sustainability, security, and affordability for a growing population. Tackling the challenges that come along with that, requires a multiscale approach where modeling results incorporating the governing physics from the smallest scale can be translated into larger, more distinct scales to understand macroscopic systems. The tool of choice to predict the underlying microscopic behavior of multiphase fluid flow in porous media is pore-scale modeling. The vast number of variables that describe chemical, thermodynamic, and mechanical effects between fluids as well as the fluids-solids interactions require computationally very expensive simulations that may take months even with cutting-edge high-performance computing. This problem raises the question if classical computers are suitable for these kinds of simulations or if other, faster computing systems might be applicable. In the last two decades, theoretical concepts describing the use of quantum computing to simulate natural phenomena have been developed and the first quantum computers have been created. In contrast to classical computers that rely on a binary system for computation and data transfer, i.e., classical bits that can either be zero or one, quantum computers make use of quantum mechanical effects such as superposition and entanglement that potentially increase the computational efficiency exponentially. Superposition means that rather than zeros and ones, bits in quantum computers, so-called qubits, can have a linear combination of both different states at the same time based on a probability-related concept of amplitudes. The second important concept is entanglement, which describes the close correlation of two quantum particles to each other independent of their location which makes it possible to mathematically compute the value of one entangled qubit by knowing the value of the respective other one. This becomes important in describing the working principle of quantum computers and how we can translate the computation results into our classical understanding for interpretation. These quantum mechanical effects are primarily responsible for the exponential increase in computational power with respect to classical computers by two to the power of n qubits (2^n). For example, to describe one of the four distinct states of a two-bit system such as 00, 01, 10, and 11, we would need the values of two classical bits, the first one to the left and the second one to the right. In order to describe the same states quantum mechanically with two qubits, we would need four values instead of two because of the principles of superposition and entanglement: a*00, b*(01+10), c*(01-10), d*11, where a, b, c, and d are coefficients. Therefore, two qubits contain four classical bits of information. This presentation introduces quantum computers and their potential applications and pitfalls concerning pore-scale modeling. It highlights methods of solving complex partial differential equations such as the Navier Stokes equation as well as discrete modeling with the Lattice Boltzmann Method quantum mechanically. Particular emphasis is made to the applicability of quantum algorithms to study solids precipitation during fluid flow in porous media with carbon sequestration applications.

Participation:

In-Person

References:

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Analysis of Effects of Minerals and Pores on Elastic and Electrical Properties Based on Multimineral and Multiscale Digital Rocks

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Electrical and acoustic properties are significant petrophysical properties. We present a comprehensive investigation of the effects of minerals and pores on electrical and elastic properties based on the multimineral and multiscale digital rocks. A novel hybrid modeling method, which combines X-ray CT scanning technique (XRCTST) and quartet structure generation set method (QSGSM), was proposed to construct multimineral and multiscale digital cores. In order to analyze the impact factors of electrical and acoustic properties, a number of synthetic digital rocks with various volume fractions of minerals and pores were constructed. By comparing the resistivity and elastic moduli of all models, it is concluded that the volume fractions of clay minerals and pores have greater effects on the electrical and acoustic properties, while quartz, feldspar, and calcite only have slight impacts on the elastic parameters and no effect on the electrical property.

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MS15 / **452**

Physics Informed Machine Learning Methods For Production Forecast

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Understanding the reservoir behavior is vital knowledge required for various aspects of the reservoir management cycle such as production optimization and establishment of the field development strategy. Reservoir simulation is the most accurate tool for production forecast, but often it is very expensive from the aspects of computational time and investment in the model building process. In this work, the machine learning methods for accurate production forecast that honor the material balance constraints are presented.

The presented approach uses two machine learning methods and one semi-analytical approach namely Capacitance Resistance Model (CRM). The first machine learning method is the powerful Generalized Additive Models (GAM) approach, which uses splines as basis functions for the representation of the solution. The advantages of splines are the smoothness of the underlying functions with continuous derivatives, and the easy way of constraining splines to monotonic and convex shapes. Another advantage of GAM is its explainability capabilities, which are inhered from the Generalized Linear Models. The second machine learning approach is a combination of Long Short-Term Memory (LSTM) and Convolutional Neural Networks (CNN), which are proven to be a good choice for time series predictions. The common extension of the two methods is the material balance constraints in the form of a CRM model, where rates are the corresponding machine learning solutions. Such constraints are necessary during the training process to avoid unphysical solutions and to honor conservation laws. The constrained GAM approach belongs to a broad category of Physics Informed Machine Learning (PIML) methods, while LSTM-CNN with constraints is part of Physics Informed Neural Networks (PINN).

The implemented approach was applied to the publicly available data with an existing history-matched reservoir model for the offshore field with several injectors and producers. This allowed us to thoroughly analyze the results of the study for communication between wells. Splines used in the GAM model have the option to be a function of one or multiple features, while Neural Networks naturally define communication between features through hidden layers and weights. Such flexibility allows taking into account inter-well connectivity, using inter-well distances, production and injection rates, and average reservoir properties, which are analogs of transmissibilities in a simulation model. The average properties are obtained through the construction of Voronoi grids around wells.

Machine learning is improving at solving difficult problems, while it often suffers from nonphysical solutions and unexplainable models. The presented machine learning methods hold the properties of explainable statistical regression models, in the case of GAM, and highly tunable time series predictors, in the case of LSTM-CNN. Both methods provide powerful predictability capabilities within material balance constraints. By no means does it try to replace the reservoir simulation but offers a complementary solution, which is reliable and necessary in cases where there is no full reservoir model available.

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Poster / 453

Evaluation of foam stability in bulk and core-scale with CO2-rich gas mixture and zwitterionic surfactants

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Co-authors: Aurora Pérez-Gramatges [1]; Juliana Maria da Fonseca Façanha [2]

[1] *Pontifical Catholic University of Rio de Janeiro*

[2] *Shell Bazil Technology*

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Foam-assisted water-alternating-gas is a promising technology to control gas mobility in carbonate reservoirs. Maintaining the stability of the foam since its generation is key to achieve this goal. It has been widely demonstrated that the high water-solubility of the carbon dioxide (CO2) favors coarsening and coalescence phenomena, negatively affecting the stability of foams formed with this gas (Farajzadeh et al., 2012). CO2-foam stability can be improved by mixing the CO2 with other less-soluble gases, such as nitrogen (N2) or methane (CH4), generating stronger foams, also improving mobility control (Siddiqui and Gajbhiye, 2017). The choice for a suitable surfactant is also fundamental for the generation of stable foams. Zwitterionic surfactants such as cocamidopropyl betaine (CAPB) and cocamidopropyl hydroxysultaine (CAHS) are good candidates for their strong tolerance to salinity and temperature, and lower adsorption on carbonate rock surface in high-salinity conditions compared to anionic surfactants. The aim of this work was to evaluate the potential of two zwitterionic surfactants (betaine and sultaine) to generate strong foams in bulk and at core-scale using CO2-rich gas mixture. Experiments were carried out under high-pressure and high-temperature (HPHT) conditions (65℃ and 10MPa) using 0.5wt% of surfactant (active matter) and 40mol% CO2 mixture with nitrogen. We evaluated foam texture and stability in bulk by sparging the gas from the bottom of the surfactant solution, and foam apparent viscosity at core-scale by co-injecting the fluids through low- and high-permeability Indiana limestone cores. Core flood experiments were performed from top-to-bottom at 3.5 x10-6 m/s Darcy velocity at varied foam qualities (fg). Bulk foam experiments showed that foams formed at HPHT were highly stable (decay of less than 10% of foam height) throughout the experiment (7200 s), suggesting that both surfactants stabilized foam despite having 40mol% concentration of CO2 in the gas phase. It was also observed that the coarsening rate obtained in bulk were similar for CAPB (6.3 mm2/s) and CAHS (6.4 mm2/s). Regarding the core flood experiments, we demonstrated that CAPB and CAHS surfactants were able to generate strong foam at HPHT using a CO2-N2 gas mixture. For CAPB surfactant, maximum foam apparent viscosity was 83 mPa.s (at fg=0.6) for the high-permeability core and 35 mPa.s (at fg=0.5) for the low-permeability core. The same parameters for the CAHS surfactant were 80 mPa.s (fg=0.6) and 13 mPa.s (fg=0.4). The formation of strong foam in porous media corroborates with the high foam stability and low coarsening rate obtained in bulk. These results confirm our observations in micromodel experiments, where we showed that using a gas mixture would improve foam texture and strength (Lopes et al., 2021) and slow down coarsening (Façanha et al., 2022). Our results suggest that the presence of CO2 as a contaminant in the gas phase would not completely destabilize foam at 10MPa and 65℃, and good mobility control could be achieved for projects with similar gas streams. Additionally, we showed that bulk experiments at HPHT correlated well with pore- and core-scale experiments, indicating that foam physical behavior could be understood across scales using these techniques.

Participation:

In-Person

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Bridging adsorption behavior of CH4-CO2 binary systems across scales

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Adsorption of CO2-CH4 binary mixtures in permeable media plays an important role in CO2-enhanced shale gas recovery and geological storage of CO2. Grand Canonical Monte Carlo (GCMC) simulations enable the examination of the physics of adsorption in nanopores with high fidelity. GCMC tracks the motion of every molecule, which results in computational expense that rises rapidly with domain size. This limits the size of computational domains that may reasonably be simulated using GCMC. The lattice Boltzmann (LB) method is, on the other hand, a mesoscopic simulation paradigm, which tracks the statistics, i.e., distribution function, of packets of molecules instead of individual ones. As such, LB may be used to bridge scales between micro-scale (atomistic simulations) and macro-scale. In this work, we use a cubic equation of state (EoS), namely the Peng-Robinson EoS, to inform the intermolecular forces in the LB framework via a pseudopotential model. This is done in a multicomponent multiple-relaxation-time LB framework where the tunable parameters are adjusted based on benchmark atomistic simulation data. We use the validated LB model to study competitive adsorption of CO2-CH4 binary mixtures in slit nanopores. These simulations incorporate intermolecular forces and the adsorption behavior under confinement and progressively examine larger and more complex media to examine the amount of CH4 that is produced while CO2 is being stored in the media at fixed pressure and temperature conditions. The results show the dynamics of adsorption in different stages of CO2-enhanced shale gas recovery and geological storage of CO2. This multiscale simulation framework helps bridge the adsorption behavior of binary systems across scales.

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Poster / **456**

Equivalent permeability estimation of vugular porous media micromodels

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Reservoir scale modelling of vuggy and fractured porous media requires upscaling and determining their equivalent permeability. The effect of vugs and fractures on single flow behaviour in porous media is still not fundamentally understood. Direct simulation models combining Darcy flow through the porous matrix and Stokes flow through vugs and fractures have been developed in recent years. This approach is computationally expensive, since the geometry configuration of vugs and fractures needs to be well described in the model. Moreover, experimental validation of the predictions is also challenging.

In this work we propose a workflow that combines experimental measurements using vugular microfluidic porous media models with different vugs configurations, solution of Brinkman formulation 1 with an extra term that accounts for the drag force generated by the top and bottom walls of the micromodel, and machine-learning methods to predict permeability of vugular porous media solely based on image of the pore structure. The relevance of the geometric features and vug connectivity taken from the binary image to the machine learning model is assessed to investigate the aspects of vug morphology that contribute to the higher observed permeability.

As a first step, the Brinkman model [2] with the drag-correction term is validated by comparing the predictions to experimental measurement of permeability of different vuggy porous media micromodel [3]. The Brinkman solver is then used to construct a training data-base with different vugs configuration, relating the geometry of the porous media to its equivalent permeability. The accuracy of the data-driven model is tested by comparing its predictions to the ones obtained by solving Brinkman model using different porous media configurations not included in the training data set. The data-driven model allows predictions of permeability of vuggy porous media at a fraction of the computational cost associated with direct simulation. The validation of the proposed workflow for single phase two-dimensional porous media allows its extension to 3D configurations and multiphase flow.

Participation:

In-Person

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MS01 / **459**

Understanding the impact of carbon mineralisation on the flow properties of basalts

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Permanent CO2 storage in basalts by means of mineralisation is a promising cost-effective way to achieving reduction of carbon emissions in view of climate change mitigation. CO2 is dissolved in water before injection in the subsurface, resulting in increased trapping safety, since solubility has already taken place. Storage of dissolved CO2 in basalts at shallow depth has additional advantages such as rapid mineralisation (1-2 years), reduced drilling and monitoring cost and lower risk of leakage and induced seismicity events. However, large-scale application of this storage technology would require substantial amounts of water making it not ecologially viable. The use of seawater as a solute is an ideal alternative that is explored since recently in Iceland. Recent studies on basalt-seawater-CO2 interaction showed that the efficiency of carbon mineralisation in seawater remains significant. Batch reactor testing revealed a total mineralisation of 20% of the initial injected CO2 within five months, corresponding to carbonation rates similar to those observed in basalt-freshwater-CO2 interaction experiments (lab and field).
Carbon mineralisation can substantially alter the pore space of the basaltic material, resulting in reduction of porosity, flow properties, and consequently overestimation of the injection and storage efficiency. While geophysical monitoring is not yet available, information on the reservoir properties of basalt remains limited. In this work, the impact of CO2 mineralisation on the hydromechanical properties of a basaltic sample is studied. For the first time, injection of CO2 dissolved in saline water is considered in view of a more ecological application of the technology at large scales. First, the flow properties of the material are measured in the lab before and after a 2-month exposure to dissolved CO2 under field-representative conditions. The experimental results show a permeability reduction of half an order of magnitude, suggesting porosity reduction due to mineral precipitation. Image analysis of x-ray tomographies of the tested sample before and after CO2 exposure show a total porosity reduction. To better understand the evolution of the pore network before and after mineralisation, pore network simulations are performed on the real 3D porosity of the material acquired from the x-ray images. Two types of porosity are considered, macro-pores and micro-pores (solid matrix porosity). Reduction of the size of macro-pores does not impact flow. To reproduce the post-exposure flow results, decrease of the solid matrix porosity is required, revealing that carbon mineralisation is more prone to take place in the micro-pores.

Participation:

In-Person

References:

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MS02 / **460**

Non-invasive monitoring of subflorescent magnesium sulfate crust formation in porous media

Author: Joseph Piotrowski[1]

Co-authors: Andreas Pohlmeier [2]; Dongwon Lee [3]; Holger Steeb [4]; Johan Alexander Huisman

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Salt precipitation from evaporation is a key factor for soil degradation in arid and semi-arid regions. Evaporation-induced water movement transports dissolved salt ions to the surface of the porous medium where they accumulate. When the solubility limit is reached, salt starts to precipitate and forms crusts on top (efflorescence) or inside (subflorescence) of the porous medium depending on the type of solute in solution. The aim of this study was to non-invasively investigate the development of subflorescent $MgSO_4$ crusts in evaporating porous media. In particular, micro-X-ray computed tomography (XRCT) was used to investigate the development of the volume fraction of precipitated salt, brine, and air and single-sided unilateral nuclear magnetic resonance (NMR) measurements were used to determine high-resolution near-surface water content profiles during evaporation. In a first step, sand packings with deionized water and $MgSO_4$ solution with an initial concentration of 0.96 mol/L were evaporated while periodically making XRCT and NMR measurements. It was found that void, brine, salt, and sand could not be segmented in the XRCT images because of limited contrast between the brine and the salt phase. However, a downward movement of the evaporation front was observed using unilateral NMR, which involved salt precipitation that deformed the top of the sand. To avoid deformation, porous sintered glass with similar porosity, intrinsic permeability, and internal surface area as the sand packings were prepared in a second step. It was found that evaporation of deionized water was similar for sand and sintered glass, which was related to the similar evaporation conditions and properties of the porous media. In contrast, evaporation of saline solution and salt crust formation differed in both porous media. The delayed crust formation in sintered glass was attributed to the smooth surface and to the highly supersaturated magnesium sulfate solution, which reduced nucleation and thus hindered crust formation. XRCT measurements on the sintered glass sample showed that salt crystals grew into the void space that was not occupied with liquid before. This suggests that film flow supported crystal growth, which needs to be analyzed in more detail in future studies. It is concluded that the surface properties of the porous medium and properties of the highly supersaturated solution (i.e., viscosity) significantly affect evaporation of $MgSO_4$ solution and the formation of subflorescent $MgSO_4$ crusts.

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Poster / 461

Hybrid Mathematical Modelling and Uncertainty Quantification of Underground Hydrogen Storage

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In order to slow the rapidly deteriorating climate crisis we need to drastically increase our use of cleaner, more renewable energy sources. Given that renewable sources are often subject to seasonal variations, the question of what to do with the excess energy has the potential to be answered by underground hydrogen storage systems. The transport of CO2 and natural gases in underground reservoir systems has been widely studied (Ma et al., 2021), however due to hydrogen's unique physico-chemical properties new problems and uncertainties arise. The storage security of underground hydrogen is largely determined by the quality of the dense porous-rock formation known as the caprock which sits on top of the storage site. To assess the potential for leakage, theoretical models need to be developed which can propagate the uncertainty in the spatially varying structure of the caprock (Ma et al., 2018) through to the macroscopic hydrogen transport dynamics. Our approach is to model the transport of hydrogen in the caprock as a diffusion-uptake process with an oscillatory boundary condition to account for the seasonal variations. We quantify the spatio-temporal variations in hydrogen distribution by modelling the diffusivity as a Gaussian random field. Using a Green's function approach (Price et al., 2022) we derive a perturbative solution for the time-averaged variance in the 1D concentration profiles of hydrogen and compare the solution to numerical approximations from Monte-Carlo simulations. Our results show that the uncertainty in the concentration of hydrogen increases non-monotonically with the correlation length of the diffusivity fluctuations. The peak variance in hydrogen concentration occurs when the correlation length is comparable to the steady-state penetration depth of hydrogen into the caprock. The predicted variance can be used to bound the uncertain concentration profile in a credible interval and our method provides a computationally cheap way to achieve this.

Participation:

In-Person

References:

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MS08 / **462**

10 years of chaotic mixing in porous media

Authors: Joris Heyman[1]; Tanguy Le Borgne[2]; Daniel Lester[3]

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In 2013, Lester et al. questioned for the first time the existence of Lagrangian chaos at pore-scale in 3D steady laminar flows through porous media. Ten years later, the ubiquity of chaotic advection has been largely demonstrated experimentally and numerically, in many porous architectures. In this talk, we review some of the main findings associated to chaotic mixing, and outline the consequences for conservative and reactive transport. We present a possible theoretical framework that allows to relax the classical macrodispersive vision of mixing and provide quantitative prediction of transport processes in porous media.

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MS07 / **463**

Numerical Simulation of Effective Models for Transport Processes in Deformable Porous Media within Mixed Eulerian/Lagrangian Framework

Author: Jonas Knoch[1]

Co-authors: Markus Gahn [2]; Maria Neuss-Radu [1]; Nicolas Neuß [1]

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We present in this talk an effective model for transport processes in periodically perforated elastic media, taking into account also cyclic elastic deformation as it occurs e.g. in lung tissue due to respiratory movement. The underlying microscopic problem consists of a linear elasticity equation for the displacement within the Lagrangian framework, posed on a fixed domain and a diffusion equation for the concentration within the Eulerian framework, posed on the current deformed domain. After a transformation of the diffusion equation onto the fixed domain, we derive the upscaled model by means of a formal asymptotic expansion. The system is nonlinearly coupled through effective coefficients, which also take into account the periodic microstructure. We develop and study numerical methods for our problem and perform simulations that are inspired by a bioengineered microdevice which is able to reconstitute critical lung functions (Lung-On-A-Chip). The simulations shed light into the sensitivity of the model with respect to several experimental parameters such as frequency or magnitude of the cyclic mechanical strain.
This is joint work with Markus Gahn (Heidelberg), Nicolas Neuß (Erlangen) and Maria Neuss-Radu (Erlangen).

Participation:

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MS09 / **464**

Direct numerical modelling of multiphase flow through reinforced porous media

Author: Luka Malenica[1]

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Understanding multiphase flow through porous media is an important study in many scientific and engineering processes. An example of such process is corrosion of steel inside reinforced porous materials, such as soil or concrete, where air-water distribution at the steel surface is directly related to corrosion mechanisms and has a great impact on durability of reinforced structures 1.
Prediction of water movement throughout unsaturated porous materials is generally based on traditional models relying on a macroscale modelling derived using representative elementary volume (REV) concept [2]. However, such models are not capable of providing detailed insight into water distribution at the steel-porous media interface which is crucial to understanding of relevant degradation mechanisms such as corrosion.
One approach that overcomes mentioned limitation of macroscale models is direct numerical simulation of multiphase flow directly at pore scale [3]. Such approach is based on solving Navier-Stokes equations where in addition to inertial, viscous, and surface forces, model accounts for interfacial tension and wall adhesion effects while fully resolving motion of the interfaces between different phases. Moreover, these models are capable to account for complex microstructure heterogeneities of real pore structures obtained by pore-scale imaging, such as X-ray microtomography or FIB-SEM techniques. Combining detailed resolution of pore-scale multiphase processes with realistic 3D geometry of pore space has large potential to improve our understanding and lead development of improved macroscale models by upscaling microscale mechanisms to obtained more accurate macroscopic properties required for practical large-scale modelling [4].
Thus, the aim of this work is to use direct numerical simulations of multiphase flow to improve our understanding of air-water distribution at interface between porous media and embedded steel. Main focus is on capillary driven multiphase flow using pore scale images with nano- to micro-scale resolution. Influence of different geometries, both synthetic and realistic 3D pore structures, as well as different flow conditions and different fluid-solid properties (gas/liquid - porous skeleton/steel) will be investigated.

Participation:

In-Person

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Poster / 465

Experimental Investigation of Wettability Alteration by Modified Salinity Water in Chalk Reservoirs

Authors: Rasoul Mokhtari[1]; Ali Talaei[1]; Louise Post Lange[1]; Sofie Nørgreen[1]; Amanda Skydt[1]; Isabelle Moraes Amorim Viegas[1]; Karen Feilberg[1]

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Wettability alteration is a widely accepted mechanism in enhanced oil recovery where modified salinity water improves oil mobilization in porous media by making reservoir rock more water wet. The equilibrium between phases in the Crude Oil-Brine-Rock (COBR) system defines the wettability state of the rock. As these properties will depend on the type of rock and crude oil it is crucial to identify each of these elements' role in the wettability alteration for a given reservoir. Contact angle measurement is an established qualitative approach to measuring the wettability state of a solid surface. In this research, we outlined a 25-1 fractional factorial design and conducted a series of dynamic contact angle measurements over 560 hours (3-4 weeks) to investigate the effect of chalk materials (reservoir and outcrop samples), brine chemistry including salinity (ranging from approximately 3000 to 50000 ppm), sulfate and magnesium concentrations (ranging from 0 to 700 and 0 to 1200 ppm, respectively), and different crude oil samples on wettability alteration. After initial contact angles were measured, 20 rock slices were aged for 4 weeks in two different crude oils at 70 ℃. Then contact angles were measured again and rock samples were distributed amongst bine samples with a varying composition according to the experimental design, at the same temperature. For the next 560 hours measurements were done in the same way at regular intervals. During the aging phase, outcrop samples showed a more marked transition to oil wetness than the reservoir samples, which indicated a higher tendency to absorb polar components from the crude oil. It was also observed that the crude oil with a higher Total Acid Number (TAN) was able to alter the wettability more toward the oil-wet state for both types of rock samples. Consequently, it was observed that the wettability modification towards water wet is more easily achieved in the rock samples aged with the lower TAN crude oil. It was also noted that wettability alteration is a complex function of brine chemistry, where total salinity and individual ion concentration play a role. It should be noted that results obtained on reservoir rock samples contradict the general understanding in the literature, which has been developed primarily based on the results on outcrop samples. These results can be used to screen suitable reservoirs for wettability alteration based on their specific rock and fluid properties. Moreover, it provides evidence that injection water can be modified to alter wettability toward water-wet to enhance oil production through imbibition and viscous force mobilization.

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In-Person

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Poster / 466

Experimental Investigation of CO2, Lean and Flue Gas Injection

in a Tight Danish North Sea Oil Reservoir

Authors: Rasoul Mokhtari[1]; Ali Talaei[1]; Karen Feilberg[1]

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Most of the Danish oil and gas is produced from Upper Cretaceous reservoirs, located in the North Sea. The rock is composed of chalk with some clay minerals as a minor impurity. Chalk is commonly considered tight, although it typically has high porosity. However, to adjust to the increasing demand for hydrocarbons, extraction of petroleum from less favorable reservoirs like the tight, high porosity low permeability mixed sediment formations in the Lower Cretaceous is needed. Lower Cretaceous oil reservoirs in the Danish part of the North Sea, are not suited to any water-based recovery method due to the depth and low permeability. The only practicable recovery method could be gas injection, and one of the targeted gases for injection could be produced gas which has good compatibility with the reservoir fluids. Another option could be the captured flue gas from industrial sites which have almost 13% CO2 content. A pure CO2 injection is also an attractive option since depleted oil and gas reservoirs are potential sites for CO2 storage projects and more CO2 will become available in the future. Therefore, this research aims to evaluate the potential of lean gas, flue gas, and supercritical CO2 injection, as well as the effect of injection pressure on incremental oil recovery in a Lower Cretaceous oil reservoir. In this study, a core plug from the Tuxen formation in the Lower Cretaceous without any open longitudinal fractures was selected after CT scanning of the core sample. To exclude the effect of rock quality on recovery results, a single core plug was re-used for all experiments. Porosity and permeability were measured before each experiment and these properties showed no change between experiments. In each experiment, the saturated core plug was aged in crude oil for four weeks under reservoir conditions (P and T). The dead oil was then displaced by live oil. The gas injection experiments afterward were conducted at two different pressures, 250 and 350 bar, at the reservoir temperature of 85 ℃. The results show that pure CO2 has the best sweep efficiency, followed by lean gas and flue gas. By comparing the pure CO2 and flue gas (Mixture of 13% CO2 and 87% N2) results, it is obvious that the high N2 content has a negative effect on final recovery. Injection pressure shows a remarkable effect on lean gas efficiency due to higher miscibility in crude oil at elevated pressure but has a minor effect on pure CO2 and flue gas results. Results suggest that CO2 injection is an attractive solution for enhancing oil recovery in tight chalk reservoirs not only because of its higher sweep efficiency but also considering its high storage efficiency and the increasing demand for CO2 storage projects.

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MS01 / 467

Insights into safe CO2 injection and storage scenarios in tight chalk reservoir samples

Authors: Rasoul Mokhtari[1]; Ali Talaei[1]; Mohammad Reza Hajiabadi[1]; Hamid M. Nick[2]; Karen Feilberg[1]

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Storing CO2 in the depleted North Sea chalk reservoirs represents a potentially attractive and cost-effective way to reduce the environmental consequences of emissions of CO2. In this study we present a comprehensive investigation of CO2 injection in chalk under different in-situ conditions which includes characterization of 1) the response of chalk to CO2 injection in the short and long term, and 2) the response of seismic measurements to various flow and mechanical alterations. The experiments are carried out on core material from a specific target reservoir in the Danish North Sea and the core plugs are saturated with relevant formation water and mounted in a pressurized injection cell at varying temperatures. Supercritical CO2 is injected into the core and the produced CO2 volume, the seismic response, and the chemical composition of the produced brine are monitored. The brine samples are analyzed for Ca2+ and other major ions in the formation brine and show the extent of calcite dissolution in the core plugs as well as other minerals being produced as a consequence of CO2 injection. In addition to the injection experiments, static experiments are presented where brine-saturated core plugs are stored for three months in contact with CO2 directly, in contact with brine in equilibrium with CO2, and with CO2 injected into the core. The core material is investigated by CT-scanning before and after the experiments and exposed to geomechanical testing to measure the extent of any rock material alteration. The knowledge gained through advanced core flooding, static exposure experiments, CT imaging, and geomechanical experiments can help to de-risk CO2 injection and storage in chalk reservoirs and will be helpful for de-risking other types of carbonate reservoirs for CO2 storage.

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MS06-A / 468

Homogenized Lattice Boltzmann Model for Simulating Multi-Phase Flows in Heterogeneous Porous Media

Author: Martin Lautenschläger[1]

Co-authors: Benjamin Kellers [1]; Julius Weinmiller [1]; Timo Danner [1]; Arnulf Latz [1]

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Abstract: Lithium-ion (Li-ion) batteries play a major role in the electrification of many business sectors as well as public and private transportation. Although being a mature battery technology, the manufacturing of Li-ion batteries has still room for optimization. A relevant example is the process step of electrolyte filling that comes with unwanted pore-scale effects such as gas entrapment. However, the underlying physics can be hardly studied using experiments, leading to the necessity of enhancing mesoscopic modeling and simulation methods.
In this context, the lattice Boltzmann method has recently gained importance for studying flow in complex porous media. It comes however at the cost of large computational expenses, especially when simultaneously simulating flow in structurally resolved pores at different length scales. Therefore, homogenization methods have been developed to circumvent the explicit modelling of pores at the smallest length scale, but describe the flow by a Darcy-Brinkman-type approach instead where only the mean permeability of the medium is considered.
In this work, we present such a homogenized lattice Boltzmann method (HLBM) that combines a grayscale approach with the multi-component Shan-Chen model. It enables simulations of multiphase flow in heterogenous porous media by physically modelling fluid-fluid and fluid-solid interactions even at sub-resolution scales. The HLBM presented here shows special advantages: the interfacial tension and wetting conditions are not affected by the homogenization and physical properties are continuous across interfaces between different porous media.
The model was validated using different test cases for single- and two-phase fluid flow. The results are in excellent agreement with the corresponding analytical solutions where available. In addition, the HLBM was applied to electrolyte filling of Li-ion batteries. On the one hand, it was used to study the influence of the nanoporous and partially permeable carbon-binder domain on the electrolyte flow. On the other hand, it was used to study flow in a fully homogenized separator microstructure with local heterogeneities.
All in all, it is shown that the HLBM can be applied to study multi-phase flow in porous media from which the pore sizes differ by orders of magnitude, without fully resolving the microstructure. This speeds up simulation times significantly. Thus, the HLBM is an efficient approach that can be applied to energy storage materials, but is not limited to it.

Acknowledgement: This work received funding from the European Union's Horizon 2020 Research and Innovation Programme within the project DEFACTO [grant number 875247]. The simulations have been carried out on the Hawk at the High-Performance Computing Center Stuttgart (HLRS) [grant LaBoRESys], and on JUSTUS 2 at the University Ulm [grant INST 40/467-1 FUGG].

Keywords: Lattice Boltzmann method, porous media, Li-ion batteries, electrolyte filling

Participation:

In-Person

References:

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Poster / 469

Nano-scale imaging and modelling of gas transport in clay-rich mudstones

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Hydrogen is considered to be a sustainable and clean energy carrier that holds significant potential to replace fossil fuels and hence enable an energy transition to meet the net-zero target set in the Paris Agreement in 2015. Large-scale underground hydrogen storage (UHS) in geological formations such as salt caverns, porous aquifers and depleted hydrogen reservoirs, can provide the predicted required scale of storage and is currently an area of focus. The sealing ability of mudstone caprocks, including marl, shale, argillite, claystone and mudstone, is a primary consideration for safe and secure storage of hydrogen, especially in the case of porous rock hydrogen storage. Additionally, an understanding of hydrogen-sealing capacity of mudstones is also important in the development of safety cases in the deep geological disposal of nuclear waste. In these systems, hydrogen gas may form due to the anoxic corrosion and degradation of steel canisters used in the underground radioactive waste repositories, resulting in the accumulation of pressure leading to rock deformation, gas migration and potential gas and other solute leakage. In both applications, therefore, hydrogen gas transport behaviour in clay nanopores is an essential parameter to understand in assessing the long-term behaviour of mudstone caprocks and seals.
Current transport models characterizing the geological transportation of subsurface fluids are not sufficient to understand the complex transport pathways and mechanisms in clay-rich rocks at nanoscale, owing to the lack of nano-scale quantitative measurement and images of the gas transport phenomenon. With recognition that 3D micro-scale X-ray computed tomography (Micro-CT) and Focused Ion Beam Scanning Electron Microscopy (FIB-SEM) commonly used for pore network modelling are insufficient to describe the clay-rich mudstones of nanometric pore sizes, Transmission Electron Microscope (TEM) can be adapted to provide microstructural information for its high magnification. This research will thus implement TEM microscopy to image the fluid's physical interactions and chemical reactions with clay-rich mudstones. Progressively, while experimental investigations of gas transport behaviours are deemed challenging in replicating the actual porous structures at a magnitude of tens of nanometres typical for clay-rich mudstones, molecular modelling with accurate established force fields describing the system's inter- and intramolecular relations in nanometre pore-scales could provide a representation of the physio-chemical coupled processes in the gas-rock system by implementing TEM imaging results as inputs.

Core samples extracted from the Lias clay formation deposited in Eastern England are adapted for common caprock representations in this study, where preliminary Scanning Electron Microscopy (SEM) tomography unveiled the microstructural pore morphologies while Energy Dispersive Spectroscopy (EDS) analyses identified numerous mineral compositions, allowing nano-scale clay specimen selection within the rock matrix. With the combination of FIB-SEM milling preparation and static TEM imaging, clay lattice fringes and pore topography were obtained for quantitative characterizations aiding future hydrogen gas transport examinations in clay-rich mudstones at nano-scale. This research thus aims to provide unique quantifications and images, hence compare with and correlate the findings to the macroscopic imaging and modelling to provide further insights for current model improvements, contributing to the new era of our energy future.

Participation:

In-Person

References:

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MS11 / **470**

Experimental study of drying in the presence of fluorescent particles in a model porous medium

Authors: Elisa Ghiringhelli[None]; Marc Prat[None]; Manuel MARCOUX[1]

[1] *Institut de Mécanique des Fliudes de Toulouse*

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The motivation for the present study stems from visualizations of the PTFE distribution in the gas diffusion layer (GDL) of Proton Exchange Membrane Fuel Cell (PEMFC). The GDL is a fibrous carbon layer treated with polytetrafluoroethylene (PTFE), by drying a layer saturated with a solution of PTFE particles, to improve hydrophobicity1. During the fabrication, internal surfaces appears to be hardly covered homogenously causing a mixed wettability in the medium, indeed PTFE distribution strongly depends on evaporation conditions2. In this context, the objective of the present work is to study the pattern formed by fluorescent particles (1μm) in porous media after the evaporation of the water.

Using a SUEX resin microchannel, we studied the effect of the presence of particles on the evaporation dynamics in a single channel3. The experiments showed that the kinematics is slowed down by the presence of the particlesdue to their effect on the thickness of the corner films. They are thicker with pure water than in the presence of particles, at small concentrations, which results in smaller vapour partial pressure gradients in the channel entrance region. Here, the work is extended considering a two-dimensional network of interconnected channels as model porous medium.

To this end, an experimental set up was developed to study the effect of the particles presence in the model porous medium, see Figure 1, and their respective deposit. The drying process is analyzed from optical visualizations, while the deposit is observed under the microscope with confocal green light.

Different parameters were varied in order to better understand the particles preferential regions of deposit and their relation with the drying pattern. For example, changing the wettability of the chip's material completely changes the localisation of the deposit. The particles concentrate in the channels closest to the top edge of the network (open edge of network), while the concentration

is decreasing further away in the network. Another variable that was changed, was the total pressure. Using an oven to perform the drying under partial vacuum condition (100mbar) and at ambient temperature, the invasion pattern is very different from the one obtained at the atmospheric pressure under diffusive evaporation condition and the deposit is more homogeneous throughout the micromodel (Fig 2).

In the next step, the experimental set-up will be improved so as to perform the experiment under a green light allowing to track the particles. This should allow us to explain how the liquid displacement influences the particle deposition Finally, it is expected that this will help establish drying procedures leading to improved GDL's hydrophobicity properties for better fuel cell operation.

Participation:

In-Person

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Poster / 471

The Uncertainty of Unsteady-State Relative Permeability Measurement Protocols

Authors: Steffen Berg[1]; Evren Unsal[1]; Harm Dijk[1]

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For the field development planning for carbon capture and sequestration and the underground storage of hydrogen, it is important to have a consistent set of relative permeability and capillary pressure-saturation functions. Regulatory requirements and minimum standards of operators may require conducting these measurements with well-established industrial protocols which have been developed over 3-4 decades, in many cases for good reasons because of the long-standing experience how non-standard workflows can result in systematic mistakes and unacceptably large uncertainty ranges.
However, because of the specific thermophysical and molecular properties of carbon dioxide and hydrogen, and a potential impact on wetting properties, ripening phenomena etc. which all potentially impact relative permeability, it may be required to perform respective measurements with the actual fluids and not with model fluids, which may be a challenge for traditional measurement protocols. For instance, in steady-state type of measurements a large fluid volume needs to be injected which can be a challenge. Although there are precedence cases where steady-state experiments for CO2 have been successfully demonstrated, the more convenient type of experiments are the unsteady-state type of experiments. However, the unsteady-state type of experiments are more difficult to interpret and the simple analytical interpretation is deceptive with respect to systematic errors and large model-based uncertainty ranges.
By using inverse modelling on a synthetic data set which serves as the ground truth, we demonstrate

how unsteady-state experiments conducted at a single flow rate and without measuring in-situ saturation profiles can result in uncertainty ranges many times larger than the instrumental error. By using in-situ saturation profiles and multiple flow rates to properly constrain the inverse model, we demonstrate that the uncertainty ranges can be reduced to that of the instrumental error, which is in the range of a few percent.

Participation:

In-Person

References:

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MS08 / **472**

Dispersion in porous media gravity currents experiencing drainage

Authors: Saeed Sheikhi[1]; Morris Flynn[2]

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We developed a theoretical and numerical model to study dispersion effects in two-dimensional porous media gravity currents experiencing drainage along their bottom boundary. The need for including dispersion comes from experimental observations of miscible gravity currents experiencing either local or dispersed drainage. In either case, it is found that significant dispersion may arise leading to the appearance of distinct bulk and dispersed phases. For the case of local drainage, we derive an analytical model starting from mass- and buoyancy-balance in both bulk and dispersed phases. The dispersion severity is characterized by quantifying the amount of fluid that appears in the dispersed phase or, equivalently, the spatial separation of leading fronts of the bulk and dispersed phases. Results for gravity currents with local drainage show that the severity of the dispersion depends on flow conditions upstream of the (local) fissure, as well as the fissure dimension and

permeability. The extension of our results to the case of distributed drainage shall also be discussed. The theoretical model is corroborated with reference to complementary COMSOL numerical simulations. COMSOL results are used to specify, in the theoretical model, the value of entrainment parameters that characterize mass transport across the bulk and dispersed phase interfaces. The COMSOL simulations are performed for various source and drainage conditions. Generally, a good agreement between theory and numerics is found.
Finally, the implications of our work to real geological flows in energy sectors i.e. H_2 storage in depleted gas reservoirs are briefly highlighted.

Funding acknowledgment: NSERC

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

473

From Infrared Light to Geomechanical Properties of Shales

Authors: Lee Jungin[None]; Olivia Cook[1]; Andrea Arguelles[1]; Yashar Mehmani[2]

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Shales play an important role in the sustainable engineering of the subsurface, both as sources of low-carbon intensity natural gas and as seals to carbon/hydrogen storage reservoirs. Their geomechanical properties are of particular interest as they allow for designing operational protocols that either prevent failure (and thus leakage) or induce optimal fracture geometries for gas flow. A major challenge is that shales are extremely heterogeneous, with spatial scales often spanning over ten orders of magnitude. Capturing this heterogeneity with any single existing instrument is not feasible, due to an inherent trade-off between resolution and field-of-view. We propose an AI-assisted hyperspectral imaging workflow, whereby geomechanical properties of shales can be mapped rapidly over hundred-meter cores with O(100 μm) resolution. The workflow relies on the hypothesis that an implicit link between infrared (IR) spectra and mechanical properties exists. Here, we validate this hypothesis for immature shale specimens from the Green River Formation and link IR spectra to acoustic velocity, acoustic scattering coefficient, and X-ray attenuation (a proxy for density). The implications are an ability to extrapolate beyond point or line measurements in the lab to scales relevant to field operations, enabling higher precision and more sustainable development of the subsurface.

Participation:

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Energy Transition Focused Abstracts:

MS03 / **474**

Shear Displacement Predictions in Fractured Rock Based on Global vs. Resolved Stress

Authors: Giulia Conti[None]; Michael Liem[1]; Stephan Matthai[2]; Patrick Jenny[None]

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Shear displacement of fractures in porous rock leads to fracture dilation influencing the flow field. This is an important mechanism in e.g. enhanced geothermal systems, where the fracture aperture determines the heat extraction performance of the reservoir. To predict shear dilation in a fractured reservoir, the shear displacement needs to be calculated first, since the dilation directly depends on it. This can be done using analytical solutions depending on far field stresses, or with mechanical solvers. Analytical solutions exist for simple test cases of isolated fractures, and approximations from far field stresses calculate the local shear and normal stress on the fracture with Cauchy's equation. However, we expect that using these two leads to wrong results in complicated fracture patterns, because the interaction between fractures is neglected. This is the main reason why mechanical solvers like boundary element methods, extended finite element methods (XFEM) and extended finite volume methods (XFVM), all of which resolve the mechanics locally by solving for stress equilibrium, were developed.

We compare results based on approximating the local stress at the fractures by the far field stress with those relying on spatially resolved stress fields obtained with a mechanical solver. While the former are computationally much cheaper, the latter are more accurate and more flexible. Our goal is to describe the accuracy and range of application of current cheap approximations regarding shear displacement. To obtain reference solutions we used a solver based on XFVM, in which the fractures are embedded manifolds of lower dimension represented by special discontinuous basis functions. These functions have the property that the displacement gradient is continuous over the fracture segments, which simplifies the computation of traction and compressive forces across the manifold. The results show that the shear displacement of a single fracture in a rock matrix is well represented by far field stress approximations. In two intersecting fractures the behavior of the fracture slipping at higher pressures is approximated well by using an adaptation depending on the fracture length. In conjugate fractures, on the other hand, the far field approximation overestimates the shear displacements. The importance of locally resolved stresses is highlighted by simulation results of a model with a layer-restricted fracture pattern mapped in the Hornelen basin in Norway, that is, large differences can be observed in the resulting aperture distributions obtained with resolved vs. global stress field approximations.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS14 / **475**

Prior ensemble based on geomechanical far-field approximations for data assimilation with ES-MDA in naturally fractured reservoirs

Authors: Michael Liem[1]; Giulia Conti[None]; Stephan Matthai[2]; Patrick Jenny[None]

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[2] *The University of Melbourne*

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The reservoir rock in subsurface applications such as geothermal or hydrocarbon reservoirs, geological carbon sequestration or nuclear waste deposition is often fractured. When fractures are present, they can potentially dominate flow and transport in those applications. It is therefore necessary to characterize the relevant fracture parameters, particularly the fracture apertures, as good as possible to reliably predict performance and assess risks. However, direct measurement of fracture parameters is difficult. Usually, only data from sparsely located wells and seismic measurements is available. Therefore, indirect methods such as outcrop analogues, geological models and production data become crucial.

Ensemble-based data assimilation is a widely used technique in subsurface applications to match production history, reduce uncertainties in model parameters and improve simulation results. In this work, we use the ensemble smoother with multiple data assimilation (ES-MDA) (Emerick & Reynolds, 2013). As an iterative ensemble smoother, ES-MDA is suited for (at least weakly) nonlinear systems (Evensen, 2018) and various studies have successfully applied it for reservoir characterization (e.g. Emerick, 2016; Ranazzi & Sampaio 2019; Todaro et al., 2021).

In this study, we use a 2D fracture geometry with more than 3500 individual fractures obtained from aerial photographs of an outcrop (Odling, 1997). We therefore assume that the fracture geometry is known a priori except for the fracture apertures. In our model, each fracture has a different aperture which is constant over the fracture length. We consider a scenario where all fractures have an initial fracture aperture which is a function of the fracture roughness. We then apply a constant far field stress, such that fractures open due to shear dilation and close due to normal stress. The exact fracture apertures are however unknown due to uncertain model parameters (e.g. fracture roughness or rock properties).

We use ES-MDA based on flow and transport data to reduce the uncertainties regarding fracture apertures and study the influence of the prior ensemble on the performance of the data assimilation framework. Calculating the individual realisations of the prior ensemble with a geomechanical simulator is expensive. A purely stochastic approach on the other hand does not incorporate all geological knowledge. As a compromise between those two methods, we propose to generate the prior ensemble based on geomechanical far field approximations which do not rely on geomechanical simulations, while geological knowledge still is incorporated to some degree. Compared to the purely stochastic approach we expect that the required number of realisations is smaller, if such a prior ensemble is employed, since it tends to be closer to the reference.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS03 / **476**

A 3D Integrated Model of Porous Media and Fractured Rock for Interpretation of Subsurface DNAPLs Migration

Author: Taehoon Kim[1]

Co-authors: Weon Shik Han [1]; Seonkyoo Yoon [2]; Peter Kang [2]; Jehyun Shin [3]; Tae Kwon Yun [1]

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Dense non-aqueous phase liquids (DNAPLs) are common organic contaminants for soil and groundwater systems, originated from industrial waste. Once disposed of incautiously, the DNAPLs migrate into the deep subsurface through different geological media. Therefore, the prediction of DNAPL migration requires specialized methods depending on the media. In this study, an integrated model that considers the different geological media including unconsolidated soil (US), weathered rock (WR), and fractured rock (FR) was developed from a detailed field investigation at a testbed in the Republic of Korea. At the testbed, various techniques of pumping tests, groundwater monitoring, and geophysical loggings and seismic surveys were implemented to represent the distinguishing feature of each geological media in the model. For example, the results of the neutron porosity logging and

core loggings were utilized for the realization of a 3D heterogeneous porosity field; the fracture properties such as orientation and aperture size were utilized to generate discrete fracture network (DFN) planes; Hydraulic connectivities of major permeable fractures detected by a series of image loggings and pumping tests were fully reflected into the model. After the process of building the integrated site characterization (ISC) model, hypothetic DNAPL transport was simulated for 100 years. The DNAPL transport and fate during the simulation time were quantitatively evaluated with the 1st and 2nd spatial moments, an indicator that assesses the spatial distribution of DNAPL mass. Additional to the base case, the evaluation for tens of cases varying the parameter in association with WR and FR conditions was conducted to perform a sensitivity analysis. As a result, the permeability anisotropy and structural differences in WR, where the greatest part of DNAPLs resided, were the most influencing factors on DNAPLs migration. They governed the location of the main fracture entrance that most DNAPLs entered, then, dramatically changes the vertical and horizontal distribution of DNAPLs in FR. In the future, the importance of each factor will be quantified and ranked by adopting a global sensitivity analysis.

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MS19 / **477**

TRANSPORT AND ENERGY CONVERSION IN NON-ISOTHERMAL BATTERY SYSTEMS. THE CASE OF THE LITHIUM BATTERY

Author: Øystein Gullbrekken[1]

Co-authors: Astrid Fagertun Gunnarshaug [2]; Signe Kjelstrup [2]; Anders Lervik [2]; Sondre Schnell [1]

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Electrochemical cells like batteries are complex heterogeneous layered structures, and each layer is frequently porous. This brings out central questions like; how many and which interfaces play a role in energy conversion? And, how do we define and measure this role? In other words, how do we describe the interplay between the various fluxes of heat, mass and charge in each layer? Most often the cell is treated as being isothermal, while this is clearly not the case when electric current is drawn. A systematic thermodynamic procedure is not only useful to model energy conversion and transport. It is needed, as current models and procedures frequently are insufficient. We have chosen to describe the energy conversion using non-equilibrium thermodynamic theory 1. This classical theory offers a consistent way to obtain flux-force relations, whether they are based on ionic fluxes and their driving forces, or on the neutral component fluxes and their conjugate driving

forces. The full set of transport coefficients can be derived directly from the entropy production 1, as well as from corresponding fluctuation dissipation theorems [2].

Using the lithium battery as an example, we first demonstrate how the various transport coefficients are interrelated [3]. We next present numerical values for a typical battery electrolyte as obtained from molecular dynamics simulations. Electrolyte models, assuming independent movement of ions, fail to capture the Onsager conductivities by a large amount. Using the solvent ethylene carbonate as a frame of reference, the co-solvent diethyl carbonate is moving across the electrolyte, contrary to current views, and create chemical potential gradients that need be overcome during operation. In addition, it is also likely that thermal gradients have an impact on battery voltage [4].

Participation:

In-Person

References:

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478

Kidney Stones Characterization Using Digital Core Analysis

Authors: Sergey Tkachev[1]; Artur Shapoval[2]

Co-authors: Gevorg Galechian [1]; Danila Golub [1]; Alim Dymov [3]; Stanislav Ali [4]; Lee Yuliya [3]; Pavel Chislov [5]; Stanislav Evlashin [6]; Julia Bondareva [6]; Anastasia Karpenko [7]; Boris Ershov [7]; Elena Popova [7]; Anastasiya Akovantseva [8]; Stuart Clark [9]; Denis Butnaru [10]; Andrey Vinarov [4]; Peter Timashev [8]

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Kidney stone disease (nephrolithiasis or urolithiasis) is a highly prevalent disease that affects up to 15% of the population worldwide. Epidemiology studies have demonstrated that the prevalence of kidney stone disease significantly varies according to age, gender, race, and geographic location, and continues to increase linearly over the last several decades. Traditional methodologies involving characterization of the uroliths involve either surface studies using microscopy or semi- or fully destructive techniques, such as thin sections analysis or X-ray powder diffraction. However, recent studies show that internal structures are the key to understanding the physicochemical interactions behind the formation and design of the future treatments of kidney stones. Furthermore, in recent years, a new paradigm called GeoBioMed, which integrates the fields of geology, biology and medicine, has emerged. The GeoBioMed paradigm involves techniques and approaches from geology such as stratigraphy or advanced imaging methods like super resolution autofluorescence microscopy or X-Ray microtomography.

In this work, we characterize three mineralogically varied urolith samples, including uric acid, calcium oxalate-monohydrate and calcium oxalate dihydrate stones, by using digital rock analysis. High-resolution 3D microtomography images of the samples were acquired and normalized to Hounsfield Units based on pre-calibrated scans. After that, images are segmented to assess and quantify resolved and unresolved pores. Next, we apply pore-network analysis to extract the morphological features of pores with respect to topology. As a result, we extract a full set of common descriptors commonly applied to reservoir rock, such as porosity, permeability, surface area, tortuosity and resulting capillary pressure curves by modelling the mercury intrusion experiment. At last, we compare these parameters with a variety of sandstone and carbonate samples.

The resulting data provides insights into the internal structures of kidney stones and the potential applications for a variety of state-of-art digital rock physics techniques recently developed to investigate the porous samples within the scopes of geo- and material sciences.

Participation:

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Energy Transition Focused Abstracts:

Poster / 479

RepoTREND –A Program Package for Safety Analysis of a Final Repository for Radioactive Waste

Author: Tatiana Reiche[None]

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RepoTREND (1,[2]) is a new simulator designed to model the processes in a final repository for radioactive waste in different geological formations. RepoTREND provides functionalities for simulating the release of contaminants and their migration through the near-field and far-field to the biosphere, including the estimation of the radiological consequences for a human and the environment. RepoTREND is modularly designed and provides computational modules for the simulation of the processes in each subsystem of a final repository.

For a typical repository model the model area is extremely heterogeneous. During a simulation of the processes in a repository for radioactive waste, numerous different effects have to be considered additionally to the basic process (two phase contaminant transport). Various physical models that use different equations and variables have to be implemented. Specific challenges in developing the structure of a simulator program are to enable a flexible choice of models for different regions of the modeled area, their combination during a simulation and an easy way to extend the program by new models and effects. The program code of RepoTREND is designed as a framework for solving a general nonlinear equation set. Different physics are realized as models in a library form.

Therefore, a model is defined by certain equation(s) of state and certain routines for taking account of the relevant effects, organized as a library of equations and a library of effects. This code structure makes it easy to incorporate new equations and effects.

Different models can be assigned to different grid blocks. Any grid block is defined by its own set of equations. The coupling of physical models is described in implicit manner: directly solve the linear couplings between variables by including all equations (block rows prepared for any grid block) in the same matrix system.

This concept ensures:
–the implementation of new effects in an easy way according to the predefined pattern,
–flexibility, transparency and reusability in extending and developing the program code.

Participation:

In-Person

References:

1 Reiche, T. RepoTREND - Das Programmpaket zur integrierten Langzeitsicherheitsanalyse von Endlager¬systemen, Report GRS-413, GRS Braunschweig, (2016) (https://www.grs.de/publikation/grs-413)
[2] Homepage RepoTREND: https://www.grs.de/en/research-development/waste-management-repotrend

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Energy Transition Focused Abstracts:

MS10 / 480

Water dynamics during gas fed CO2-electrolysis revealed by 4D X-ray imaging

Authors: Robert Fischer[1]; Matthieu Dessiex[2]; Federica Marone[3]; Felix N. Büchi[1]

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CO2-electrolysis (CO2ELY) is a promising technology to harvest the temporal surplus of renewable energy and convert CO2 into valuable non-fossil feedstock for green chemistry. CO2ELY is similar to water electrolysis. CO2-gas is fed to the cathode to be electrochemically reduced, e.g. to CO, with an adapted catalyst. We employ time-resolved synchrotron X-ray tomographic microscopy (XTM) to study operando the complex water dynamics during CO2ELY and its relation to electrochemical performance. Water plays an essential role as a reactant for the CO2 reduction reaction (CO2RR) in alkaline conditions, while condensed water can block gas exchange in the gas diffusion layer (GDL). Water is further involved in the process through vapor adsorption/desorption, capillary fingering in the GDL and hygroscopic swelling of the polymer electrolyte membrane.
A zero-gap electrolyzer with a bipolar membrane (BPM) in forward bias 1 - alkaline at the cathode, acidic at the anode - is studied. The membrane is sandwiched between two porous electrodes based on carbon paper GDLs. The cathode GDL additionally carries a microporous layer. This membrane electrode assembly is clamped between two polar plates containing flow channels for gas and water at the cathode and anode, respectively. A custom-made miniature electrolyzer with an active area of 10 mm2 is used for XTM [2]. This miniature cell is mounted on the rotating sample stage of the TOMCAT beamline at the SLS, Paul Scherrer Institut, Villigen PSI, Switzerland. During electrochemical operation, fast tomographic scans (1s/scan) of the active region are recorded every minute for 45 min with a voxel size of 2.75 um. The concurrent electrochemical performance is measured and related to the liquid water evolution and gas bubble formation within the cell. Beyond qualitatively correlating the imaging results to the electrochemical data, the different phases in the image data are segmented to study the evolution of the liquid water configuration in detail. Due to substantial deformation of the sample during acquisition, i.e. strong membrane swelling with GDL compression, differential segmentation methods are not applicable. We extend machine learning segmentation (e.g. Weka [3], usually 2D) to exploit information in all four dimensions at once.
Imaging reveals the multilayer system of 0.8 mm-wide flow channels, GDLs, microporous layer, catalyst layers and the BPM, particularly resolving the inter-fiber GDL-pores in the range of 20 um. The temporal resolution allows tracking the evolution of liquid water. It is a delicate balance between feeding the CO2RR with reactant water and not blocking the gas transport. Water condensation is observed in the GDL and, more severely, creates blocking slugs in the flow channels at the cathode. Additionally, hygroscopic swelling of the membrane together with catalyst delamination and BPM-interface fracturing is observed.
The presented experimental results help to better understand water dynamics during CO2-electrolysis to ultimately yield higher power density and stability. The results further reveal important degradation processes, particularly in the BPM. The combined electrochemical and imaging data can further inform modeling to accelerate the search for optimal operation parameters.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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Poster / 481

Modelling surface-washing of porous media: dye-attenuation of a passive tracer

Authors: Francesco Paolo Conto'[1]; Emily Butler[2]; Merlin Etzold[3]; Julien Landel[4]; Stuart Dalziel[1]

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The cleaning and decontamination of various porous surfaces (e.g., concrete, tarmac, wood, etc.) is a challenging and multidisciplinary problem for both fundamental understanding and a wide range of industrial, medical, urban, everyday-life and disaster-response applications 1. The role of such processes is particularly crucial in cases where contaminants (such as chemical substances and biological pathogens) are extremely harmful and pose serious risks to human health. Indeed, attempts to decontaminate porous materials might lead to a partial redistribution of the unwanted substance within the porous matrix instead of a complete removal. As a result, cleaning operations could further contribute to the contaminant/pathogen spread, and the substance might remain a long-term hazard for people coming in contact with the contaminated medium.

In this work, we present surface-washing experiments modelling the decontamination of porous media using a rig equipped with camera-based (spatially resolved) and in-line UV-Vis diagnostics.

The model porous surfaces used are manufactured in our laboratory by sintering packings of soda-lime glass beads of various size distributions onto solid glass frames. The obtained composite structures are then directly incorporated in a surface-washing apparatus [2].

The contaminant agent is simulated by a dyed passive tracer, either disodium-fluorescein or methylene blue. These aqueous solutions are released onto the free porous surface of a water-saturated medium in the form of droplets. The surface-washing is simulated by a thin gravity-driven water film flowing over the inclined porous-glass plane.

The space-time evolution of the contaminant field across the porous medium and its interaction with the cleansing flow are then tracked by direct image analysis based on dye-attenuation using multi-wavelength illumination spectra. This technique enables us to study the tracer spreading (advection, diffusion, dispersion, and absorption) over a wide range of concentrations. Additionally, an inline UV-Vis spectrometer is used to monitor in real-time the contaminant concentration in the washing effluent.

Our experiments provide insights into the fundamental physics governing the cleaning process, such as the role of initial conditions (e.g., ingress of contaminant, wet/dry substrate) and the impact of process parameters on the decontamination efficiency (e.g., necessary amount of cleansing resources and washing time). Importantly, they demonstrate a decontamination-induced redistribution of the contaminant within the porous matrix.

Finally, we provide some fundamental considerations regarding the choice of the optical method in

a dye-attenuation context. In particular, we discuss how the factors such as the light source, the dye absorbance, the camera-response, and the medium void-fraction distributions complicate the accurate tracking of the contaminant simulant.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS07 / **482**

Upscaling investigations of dissolution using machine learning and GeoChemFoam

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[1] *Heriot-Watt University*

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Dissolution of solid mineral in porous media due to the introduction of reactive fluids is of utmost importance for a wide range of subsurface applications, including CO2 storage, geothermal systems, fuel cell technology, and enhanced oil recovery. The conditions of the injection process as well as the mineral properties strongly influence the resulting dissolution pattern, leading to compact, uniform, wormholing, or channeling dissolution that change the permeability and flow properties of the reservoir. In this work, we present a comprehensive analysis of the impact of pore-space heterogeneity on the various regimes during acid injection at the pore-scale using numerical simulation. Our fast, efficient dissolution numerical model, based on the Darcy-Brinkman-Stokes method within the OpenFOAM toolbox in GeoChemFoam, is used to run 2D simulations of dissolution on ultra-large synthetic, stochastically created geometries with varying levels of pore-space heterogeneity. For each model, the influence of flow and reactive conditions on the local dissolution is characterized. We observe that heterogeneities in the pore space facilitate the development of local flow instabilities that result in wormholes and channels due to the existence of preferential flow paths. These flow and reactive parameters are extracted with mage analysis and used to train a deep neural network to predict the porosity and permeability changes on Darcy-scale grids. This is the first work to directly compare pore and Darcy scale model results for reactive dissolution systems, giving insight into the interplay between flow, reaction, and heterogeneity across scales.

Participation:

In-Person

References:

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MS11 / **483**

Capillary-controlled phase transitions in caprock over CO2 storage in aquifer simulated by nanofluidic pore models

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CO2 injection in deep aquifers is a way to perform CO2 storage, but it requires an impervious overlying formation called caprock to avoid any catastrophic leakage. The post-injection CO2 bubbles accumulate rapidly at the aquifer-caprock interface, creating a multiphasic situation and drying the caprock interface. Due to the thinness of the pore size distribution, this drying can lead to the formation of nanoscale capillary bridges, meaning that the entire water-bearing caprock is put in a capillary state, i.e., liquid under negative pressure (tension) [1, 2]. Therefore, the evolution of geochemical reactions and the dynamics of liquid-air partitioning must be capillary-corrected.

To study the capillary-driven mass balance and its associated geochemical features, capillary water bodies were experimentally investigated within synthetic lab-on-a-chip pore models with perfectly controlled inner geometries. As shown in Fig.1, these experiments are carried out using nano/microfluidic chipsets designed based on two feeding micro-channels connected by a series of nano-channels. These nano-channels, etched in a silicon wafer, have a depth varying from 5 to 100 nm and allow us to control or change the capillary states and relative humidity (RH) of a flowing aqueous solution of known composition.

The capillary features of the solution were investigated by employing the 5 nm depth channel and tuning the relative humidity at 50% (capillary evaporation) and 80% (very close to capillary equilibrium). We observed that water boiled in the big reservoir (micro-channels) behind the nano-channels after 60 days at 80%, while no significant evaporation was measured. Meanwhile, permanent capillary evaporation occurs in nano-channels maintained at 50%, and the corresponding kinetic rate was measured. These experiments give insights into the coupling between pore-size-controlled and capillary-controlled geochemistry in porous media, which will be discussed.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 485

Stress concentration in the local load sharing fiber bundle model

Author: Elias Lundheim[1]

Co-authors: Alex Hansen [1]; Jonas Tøgersen Kjellstadli [1]; Santanu Sinha [2]

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Material failure and fracture growth are phenomena that without a doubt have significant impact on industry and society alike. They dictate how long structures will last and what loads they can withstand, critical topics to consider in any engineering project. While some analytical formulations have shown partial success in describing and predicting material failure, numerical studies of Fiber Bundle Models (FBM) and Random Fuse Models (RFM) have given many interesting results, and are still frequently used in research today 1. The fiber bundle model represents materials as a system of Hookian springs that break when critically stressed. A 2D fiber bundle is similar in structure to a cross section of a pours material, and while many explore flow through capillary fibers [2-4], others study the mechanical strength [5-6]. Global Load Sharing (GLS) is a type of fiber bundle where all the fibers in the bundle carry the same amount of load. This is similar to what would happen if a perfectly rigid material is stressed. However, if a material is flexible, the load will be focused more locally. In such a situation, Local Load Sharing (LLS) is more appropriate. To give some physical intuition of these extremes of GLS and LLS, consider eating a cake with a spoon. The cake is flexible and breaks locally around where the spoon is pushed through the cake. Compare this to what might happen if you use the spoon to try to take a piece out of a brittle cracker. There would be no spoon shaped hole in the cracker, because the stress from the spoon would not remain local, but be distributed globally. LLS has properties similar to that of a soft materials where as GLS is more similar to hard materials. Keep in mind however that soft/hard is different from elastic/brittle and that both GLS and LLS are capable of behaving elastically and brittley. The way LLS distributes load onto fibers is by grouping adjacent broken fibers in to groups called clusters. The fibers on the perimeter of each cluster are then given the load that would have been carried by the broken fibers in the cluster. This behavior leads to crack growth, as large clusters are more likely to grow even larger because their perimeters are stressed as a function of cluster size. This study explores a new way to distribute the load in the bundle that further elaborates on the idea of crack propagation. Our method, first suggested by Kjellstadli [7], is closely related to LLS but uses a non-uniform load distribution over the perimeter of clusters. LLS already has a mechanism for crack enhancement, but our method targets fibers individually as opposed to entire perimeters. We let fibers with fewer neighbours take on more load than fibers with more neighbours. Our implementation is a generalized model that contains LLS as a limit. When tuning the model away from LLS, the model produces clusters that are more solid, as opposed to the more fractal clusters commonly seen in LLS.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS18 / **486**

Modeling dehalogenation of diatrizoate by sulfide-modified nano-scale zero-valent iron in natural porous media.

Authors: Angeliki Koupa[None]; Monica Riva[1]

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Iodinated Contrast Media (ICM) are organic compounds, widely used during X-ray procedures for medical imaging 1. ICM are connected with diseases, such as hyperthyroidism or hypothyroidism, due to the iodine ions bound to the chemical molecule [2]. Moreover, in aquifer system, ICM can form toxic intermediate products during photodegradation or Managed Aquifer Recharge processes 1.
Nano-scale zero-valent iron (nZVI) can efficiently dehalogenate ICM and turn ICM into non-toxic products 1. The chemical reaction between ICM and nZVI is impacted by several factors, such as the initial concentration of nZVI, the presence of oxygen in the subsurface environment (i.e., the occurrence of anaerobic versus aerobic conditions) and the pH of fluid phase. Although several experimental studies have analyzed the reaction kinetics between ICM and nZVI at laboratory scale under batch conditions ([3],[4],[5]), few studies have investigated the interaction between ICM and nZVI under flow conditions. In this framework, Zhou et al. [6] performed both batch and column experiments in order to identify the reaction mechanism and kinetics of diatrozate (DTA) dehalogenation using sulfide-modified nZVI (S-nZVI) under anaerobic conditions. The authors also proposed a pseudo-first-order kinetic model to interpret the batch experiment outcomes. However, the proposed model cannot adequately reproduce the experimental results obtained under flow condition.
Here, we cast the batch experiment of Zhou et al. [6] within a stochastic framework and (i) provide Maximum Likelihood estimates and associated uncertainties of characteristic parameters driving the underlying kinetic mechanisms and (ii) assess the way uncertainty associated with model parameters

propagates into uncertainty in quantifying the temporal evolution of DTA concentration. Finally, we propose a new kinetic model able to describe the interaction between DTA and S-nZVI under flow conditions. The new kinetic model which includes advective-dispersive transport, sorption and desorption to and from the reactive surface (S-nZVI), dehalogenation of DTA by S-nZVI, adequately reproduces the experimental results.

Participation:

In-Person

References:

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MS08 / **487**

High Resolution Mixing and Reactions in a Porous Column

Authors: Saif Allah Farhat[1]; Daniel Hallack[1]; Guillem Sole Mari[2]; Diogo Bolster[1]

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We use high resolution numerical direct numerical simulations to study flow and transport in a full length porous column, solving the Navier-Stokes and advection-diffusion equation to fully resolve all processes at pore scale. The data is used to take a very close look at interfacial and mixing processes at unprecedented resolution, enabling us to accurately track mixing interfaces, quantify incomplete mixing and reactions and study boundary effects to gain a deeper understanding of the origin of anomalous behaviors that cannot currently be measured in laboratory experiments.

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Energy Transition Focused Abstracts:

MS06-B / 488

Recent Advances in Modelling Reactive Interfaces in Pore-Scale Simulations

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[1] *CNRS Orleans, Univ Orleans*

[2] *Heriot-Watt University*

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Micro-continuum modeling enables the simulation of coupled multi-physics processes including multiphase flow and reactive transport at the pore scale. One key feature is the ability to move fluid-solid (e.g. mineral dissolution or precipitation) and fluid-fluid interfaces (e.g. dissolution of gaseous species in aqueous phase) using fixed-grids only, i.e without the need to remesh the grid when the mapping of phases evolves. The displacement of such interfaces relies on an accurate description of mass transfer between the two phases. Various approaches have been proposed to model, on the one hand, the reactive mass transfer at the solid surface, and on the other hand the transfer of species across the interface between two immiscible fluids. In this presentation, we discuss the recent progress made to simulate such processes under thermodynamic equilibrium and non-equilibrium. We review the Continuous Species Transfer techniques, the Volume of Solid approaches, and we introduce a new tentative to combine these two models into a unique framework.

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In-Person

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Energy Transition Focused Abstracts:

MS01 / **489**

Effects of Thermal Shocks on Cement for CCS under Confined and Unconfined Conditions

Authors: Kai Li[1]; Anne Pluymakers[1]

[1] *Delft University of Technology*

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In wells for carbon capture and storage (CCS), fractures can develop in the cement due to strong thermal shocks upon pressurized CO2 injection into the subsurface. The network of these fractures forms leakage pathways that can impair well integrity, and thus impede successful geological storage of CO2. In this study, we investigate how thermal shocks affect cement integrity under unconfined and confined conditions. Solid cylindrical samples (Φ3 x 7 cm) and samples of the same size but with a hole (Φ4 mm) in the middle are used. All samples are prepared using class G cement with 35% BWOC silica flour by Halliburton AS Norway, in accordance with API specification 10B-2. In unconfined experiments, we either quench the solid sample into cold water or inject cold water through the hollow-cylindrical sample to induce thermal shocks. In confined experiments, we mount the hollow-cylindrical sample in a triaxial deformation setup with confining pressure and axial stress, then inject cold water to induce the shocks. Before the shocks in all experiments, samples have been heated to 130℃. The temperature of the water is 5℃ to achieve a strong thermal shock as possible. We produce eight cycles of thermal shock in all experiments. To study the extent of cracking, we use a micro-computed tomography (μ-CT) scanner to characterize the network of pores and fractures in the cement before and after experiments.

Under unconfined conditions, fractures develop in cement after thermal shocks in both quenching and injecting-through experiments. Both experiments generate sufficient thermal stresses to cause cracking in cement. In quenching, multiple fractures are initiated at different orientations. However, by injecting cold water through the sample, only one longitudinal fracture is created. This fracture is intersected with the injecting hole, where most thermal stresses are built up. The volume ratio of pores and fractures in samples increases to 2.74% by quenching and 1.84% by injecting through respectively, from 0.38%. Compressive strength decreases from 97.9 MPa for intact samples to 53.9 MPa after quenching, and 83.6 MPa after the injecting-through experiment. Under confined conditions, we carry out injecting-through experiments to bring about thermal shocks under 1.5 and 10 MPa confining pressure. We haven't observed any failure in cement integrity under either confinement. Instead, compressive strength increases by 6.2% and 7.2%, and the volume ratio of pores and fractures decreases by 7.7% and 18.2% after the experiment under the confinement of 1.5 and 10 MPa, respectively. This means the presence of confining pressure not only hinders the adverse effects of thermal stresses on cement integrity but also compacts the samples. Higher confining pressure causes more compression to the sample, then resulting in greater strength.

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Poster / 490

Fast workflow to estimate petrophysical properties: From Digital Rock Physics Scale to Laboratory Scale

Authors: Marco Miarelli[1]; Leili Moghadasi[1]

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Petrophysical rock properties (i.e., porosity, absolute and relative permeabilities) are key information for any reservoir characterization and represent fundamental input parameters for the simulation studies. To access to such information typically core analysis are needed. Although core analysis tests are an accurate way to obtain such properties (Gaafar et al. 2015), there are cases where these tests are not accomplished or not profitable to oil companies. Firstly, laboratory experiments can take a long time to be completed. Secondly, core plugs can be scarce, damaged or unsuitable for the tests. Recently in order to obtain reliable petrophysical properties from core plugs even when they are no longer suitable for laboratory experiments, digital rock physics techniques (DRP) may represent a as a powerful approach to obtain these parameters. DRP has progressed at rapidly and is becoming an indispensable tool for rock physics analysis even if the comparison between DRP results (micrometric scale) and laboratory tests (centimetric scale) needs the implementation of an additional upscaling method. DRP investigates the physical fluid flow properties of porous rock combining modern macroscopic imaging with advanced numerical simulations. The implementation of an upscaling method is required to validate DRP results (micrometric scale) and laboratory tests (centimetric scale). In this context, we propose a novel methodology (Miarelli and Della Torre 2021) allowing the digital characterization of rock properties at the plug scale. In particular, the developed workflow valorizes and combines different technologies (Figure 1): (i) micro-CT scan, (ii) advanced image processing, (iii) machine learning (Menke et al. 2021, Jouini et al. 2021), (iv) Computational Fluid Dynamic (CFD) numerical simulation. The first step of the methodology consists of acquiring micro-CT low-resolution scan of the entire core plug; then, machine learning techniques are applied to decompose the digital plug (derived by image processing on micro-CT scan) in reference element of volume(REV)-type equivalent blocks, determining the optimum number of REV type and their locations. One or several high-resolution 3D fine-scale images are used to derive the petrophysical properties of each REV type from individual fluid flow simulations at the pore scale. The resulting REV-type properties are then scaled up to the core plug scale. Finally, the scaled-up results are compared to the results of core analysis tests. The overall methodology is validated on a heterogeneous carbonate rock.

The structure of the implemented workflow allows to improve every single step to adapt the procedure to every different core plug rock types. In this sense, the developed workflow could be further upgraded in several ways. From the detection side of texture analysis, increasing REV attributes number, including spatial point process (Weil et al.2006), could better cluster analysis results. Optimal value for clusters number can be investigated adopting supervised machine learning technique instead of unsupervised ones. The developed workflow can be expanded to two-phase flow properties, using volume-of-fluid(VOF) approach, in order to evaluate relative permeability and capillary pressure of drainage and imbibition processes (Heyns and Oxtoby 2014;Brackbill et al. 1992;Shams et al. 2018) by an accurate modelling of low capillary or tension surface-dominated flows.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 491

Water-H2-Quartz and Water-H2-Calcite Wettability Measurements: An Experimental and Theoretical Investigation

Authors: Ahmed Al-Yaseri[1]; Safwat Abdelazeim[1]

[1] *King Fahd University of Petroleum and Minerals*

Corresponding Authors: ahmed.yaseri@kfupm.edu.sa, abdelazeim@kfupm.edu.sa

Sandstone and carbonate H2-wettability is an important factor that defines structural and residual trapping capacities and significantly influences multi-phase fluid dynamics in the rock. An increasing number of studies have evaluated this wettability by performing contact angle measurements on quartz and calcite; however, the reported data is fraught with uncertainty.
We show clearly that surface contamination is the main cause of this widespread data dispersion. Incorrect cleaning methods were used, resulting in falsely high contact angle values. We used the surface cleaning method commonly used in the surface chemistry community to observe that in the presence of hydrogen, the water contact angles on clean quartz and calcite substrates are zero in all conditions (i.e., different pressures, temperatures, and salinities) using the sessile drop method and Molecular Dynamics (MD) simulation.

Participation:

In-Person

References:

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493

Experimental Investigation of Oil Recovery Mechanisms Using Water-wet and Mixed-wet microfluidic devices

Author: Abdullah AlOmier[None]

Co-authors: Antonia Sugar [1]; Dongkyu Cha [2]; Subhash Ayirala [2]; Mohammed AlOtaibi [2]; Ali A. Yousef [2]; Hussein Hoteit [3]

[1] *King Abdullah University of Science & Technology*

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Objectives/Scope:
Assessment of the recovery mechanisms in mixed-wet systems, such as carbonate and shale reservoirs, has gained a significant attention by the industry. Wettability of oil-brine-rock systems is a crucial petrophysical property that impacts fluid distribution and multiphase flow in hydrocarbon reservoirs. Microfluidics is a unique technology that can provide direct visualization and assessment of flow mechanisms at the pore scale. However, mimicking mixed-wet systems becomes a limitation to this technology. In this work, we investigate the influence of wettability on oil recovery using microfluidic devices mimicking formations with single and mixed wettabilities for the first time.
Methods, Procedures, Process:
The microfluidic devices were designed to replicate the actual pore-network of an oil-bearing reservoir rock, obtained from thin-section images of a core. The microdevices were built out of silicon due to their compatibility with organic solvents, such as oil. A novel technique was used to construct the microfluidic substrates with controlled wettability, including water-, and mixed-wet systems, imitating pore-network formations with variable pore-throats.
Results, Observation, Conclusions:
Several sets of comparative experiments were performed to investigate the wettability effect on oil recovery at the pore scale. Fluid flow was conducted in two silicon-based microfluidic devices holding the same pore-network structure but differed in the wetting state. The first microdevice had a hydrophilic silicon-based surface which did not undergo any surface modification processes, mimicking a water-wet system. While the second microdevice underwent selective wettability alteration by depositing perfluorodecyltrichlorosilane (FDTS) on selective zones of the silicon-based micromodel surface. This created multiple hydrophobic spots on surface, mimicking a mixed-wet system. The flow experiments conducted shared identical conditions: water injection in oil-saturated microdevices. Results showed a reduction in the oil recovery and thus a higher remaining oil saturation in the mixed-wet compared to the water-wet microdevice with distinct phase distributions. The results highlight the importance of using accurately designed microdevices to mimic mixed-wet formations when evaluating oil recovery, as single-wetting state microdevices may under-, or over-estimate the recovery process.
Novel/Additive Information:
This work presents an assessment of oil recovery mechanisms in mixed-wet systems using microfluidic devices. Microfluidic devices with mixed selective wettability using FTDS coating to alter the substrate surface are demonstrated for the first time. Tuning the wetting state of the microdevices to mimic the mixed-wet characteristics of reservoir rocks can enhance the understanding of multiphase flow behavior and recovery mechanisms in mixed-wet reservoirs, including carbonates and shales.

Participation:

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Poster / 494

Inelastic deformation of porous sandstones and its influence on rock properties under cyclic triaxial loading conditions

Author: Ming Wen[1]

Co-authors: Andreas Busch [1]; Nick Harpers [2]; Kamaljit Singh [2]; Jim Buckman [2]

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In underground hydrogen storage, pore pressure cycling due to annual or more frequent gas production (depletion) and injection leads to changes in the stresses acting on the reservoir rock, which in turn lead to rock deformation. Although inelastic deformation has an important effect on the physical properties of the rock, its effect on rock mechanical and transport properties is not well understood. To investigate the effect of inelastic strain, triaxial cyclic axial compression experiments were carried out on Castlegate and St Bees sandstone samples with 26% and 20% porosity, respectively. This was done using the Harpers THMC Flow Bench at Heriot-Watt University at 4.5 MPa, 10.5 MPa, and 19.5 MPa confining pressure. Permeability tests were carried out at key differential stress points throughout the compression tests. 3D images of the whole specimens before and after the cyclic loading experiments were obtained by performing X-ray micro-computed tomography scans, and digital core models were established to quantitatively characterize the geometric topological features of the two sandstones. The results show that the total axial strains of the two sandstones after cyclic loading ranges from 0.98–1.42% and 0.82–1.17%, respectively. The more porous Castlegate sandstone shows greater inelastic strain than the St Bees sandstone (0.47 to 0.85%, compared to 0.23–0.62%, respectively). However, upon stress changes, the Castlegate permeability shows lower permeability loss (19-46%) compared to St Bees Sandstone (~70%). In both sandstone samples, the first cyclic loading event produced the most significant inelastic strain and therefore permeability loss. Microstructural evidence based on CT analysis indicates that inelastic compaction in the Castlegate sandstone is controlled by a combination of intergranular cracking and intergranular slip, with the former dominating. Some of the large pores were compacted to form smaller pores due to intergranular slip, causing a decrease in the permeability of this sandstone, and the inelastic compaction became more pronounced as the confining pressure increased. In contrast, for the St Bees sandstone, inelastic compaction is mainly controlled by intergranular and intra/transgranular cracking. In addition, broken grains in the pores and throats were responsible for the decrease in permeability.

Participation:

In-Person

References:

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MS03 / **495**

A six (+1) field formulation for flow in porous media with fractures and barriers

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[1] *Politecnico di Torino*

Corresponding Author: stefano.scialo@polito.it

A domain decomposition approach for flow simulations in poro-fractured media using non-conforming meshes is presented. Fractures in a porous medium can either act as preferential flow path, either represent barriers for the flow. When a geometrical reduction approach is used, as, e.g. in a Discrete Fracture and Matrix (DFM) model, fractures are represented as planar interfaces embedded in a three dimensional porous matrix. A formulation with six independent pressure variables and an additional field for the flux at fracture intersections is proposed to de-couple the problems on each fracture and in the bulk domain. A suitable cost functional is then minimized to recover the global solution. Each field can be discretized independently from the others, and on an independently built mesh. As the pressure solution in the porous matrix can be discontinuous across barrier interfaces, the eXtended Finite Element method with discontinuous enrichment functions is used to describe this kind of irregular behavior on a mesh non conforming to the irregularity interface.
The proposed approach has the advantage of a strong robustness to geometrically complex configuration and allows to take advantage of parallel computing techniques.

Participation:

In-Person

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Energy Transition Focused Abstracts:

496

Magnetic Resonance Imaging for the Characterization of Local Particle Wetting inside a Slender Trickle Bed Reactor

Authors: Ali Fathiganjehlou[1]; E.A.J.F. (Frank) Peters[1]; K.A. (Kay) Buist[1]; J.A.M. (Hans) Kuipers[1]

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A trickle bed reactor (TBR) is one of the most common reactor types in the chemical and petroleum industries. A TBR accommodates a catalyst particle packing with two-phase gas-liquid flow moving co-currently downward. The catalyst particles provide a large surface area for sufficient contact of the liquid and gas phases containing the reactant. A proper distribution of the gas and liquid among the catalyst particles will provide the desired particle wetting efficiency, which is essential for the optimal operation of a TBR. This becomes more important in slender TBRs, i.e., low column-to-particle diameter ratio. Slender TBRs are favorable when proper heat control over the reactor is required. The small column diameter in the slender TBR highly affects the gas-liquid distribution and causes the liquid and gas flow to move through preferential regions. Therefore, a detailed understanding of the local phase distribution and particle wetting is crucial in designing a slender TBR. This research uses Magnetic Resonance Imaging (MRI) to characterize the gas-liquid-solid distribution and the particle wetting efficiency for a two-phase trickle flow inside a slender TBR of 21mm inner diameter randomly filled with 3mm mono-disperse spherical particles. The 3D liquid distribution images from single-phase and two-phase flows are obtained using a 3D Fast Low Angle-Shot (3D FLASH) imaging sequence of MRI. The acquired images are post-processed to calculate the local saturation field and wetting area fraction of each particle. It is investigated to see if preferential flow in a slender TBR could lead to a preferential local wetting of the particles' surface.

Participation:

Online

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MS03 / **497**

Physical models for fracture flow tests by 3D-scanning and -printing

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Visual observation of flow and transport processes in fractures require transparent replicas. Quite easily realized are parallel plate models which pose only a quite rough approximation and require

certain geometric conditions /TSA 87/. A better representation can be gained by impressions from real fractures, either by forming the free space, a common technique (e.g. /PER 95/) but rather effortful, or by epoxi imprints of the fracture surfaces (e.g. /WIN 20/). Accurate surface measurements and determination of contact pressures indicate, though, that several imprints of the same locations may show significant differences /STI 20/.
A rather new class of transparent physical models has been made possible with the introduction of reasonably accurate 3D-printers. Hydraulic tests with principle models of single fractures as well as DFNs have been established quite early (e.g. /ISH 19/, /SUZ 17/). Realistic single fracture replicas still pose a problem, though.
Three steps are required for the production of a fracture replica by this method:
1. 3D-scanning of the fracture surfaces
2. Preparation of a printable digital model of the fracture
3. Printing out the digital model
This procedure has a lot of appeal as it rather elegantly avoids the problem of air enclosure and bubble evolution between resin and fracture surface. Moreover, it is possible to add features to the digital model that facilitate hydraulic tests such as connectors to inflow and outflow tubes. The method allows even for repeating destructive tests. Since it was intended to cover the whole production process of this method, a 3D-scanner as well as a 3D-printer have been acquired accordingly.
However, new challenges appear also at all three stages of production. One obvious point is the accuracy. The coordinates of a fracture surface can of course only be sampled at a limited number of scanning points. On the same scale, also the dimensional accuracy of the 3D-Printer is restricted. Less evident is the problem of alignment of the two fracture surfaces. Snapping points at a distance of less than one millimetre have been found in a printed fracture of a 7 x 10 cm size, suggesting a possibly serious impact on the aperture distribution by misalignment. Another point concerns the general ability of plastics to take up water. This phenomenon affects printed resin material to a considerable extent in that weight and size change with time. Details and solutions to these problems are addressed in the present paper.
In closing, the repeatability of an actual tracer test in a printed fracture replica is investigated. The experimental setup consists of an upper and a lower part. Transport of a colored solution in the fully water-filled replica has then been observed with an industrial camera and repeated three times. Grayscale images were acquired every 10s. The post-processing includes a segmentation of each image and a statistic evaluation for all pixels. This statistic provides information for each pixel stating with which probability there was tracer measured at this spot or not.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS03 / **498**

Impact of matrix diffusion on heat transport through heterogeneous fractured aquifers

Authors: Silvia De Simone[1]; Olivier Bour[2]; Philippe Davy[2]

[1] *Institute of Environmental Assessment and Water Research (IDAEA-CSIC, Spain)*

[2] *Geosciences Rennes, UMR 6118 CNRS/Universite de Rennes I*

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In this study, we illustrate key features of transport in heterogeneous fractured aquifers, when the fluid-rock diffusive exchange is a significant player, like in the case of heat transport. This advective-diffusive behavior is determined by the combined effects of flow velocity heterogeneity in the fracture system, and diffusive exchange between the fluid in the fractures and the rock matrix. In this context, the temporal evolution of the response to a pulse injection exhibits a post-peak pre-asymptotic regime, with a slope that deviate from the traditional signature of matrix diffusion. This deviation is driven by the variability of both velocity field and fracture aperture field. We illustrate the impacts of these two factors, under different conditions of heterogeneity and fracture network connectivity. We derive theoretical models that predict the pre-asymptotic tail under three extreme cases that can be related with specific network structures, i.e., networks dominated by large or small fractures, networks with highly or poorly channelized flow. These theoretical predictions are compared with results from numerical simulations in different sets of three-dimensional discrete fracture networks. Based on the numerical and theoretical results, we determine that the combined observation of solute and heat transport responses allows classifying the network in terms of connectivity structure, and partially characterizing the fracture aperture variability in terms of upscaled parameters.

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In-Person

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MS17 / **500**

On talik formation related to geological radioactive waste storage

Author: Klaus-Peter Kröhn[1]

[1] *GRS gGmbH*

Corresponding Author: klaus-peter.kroehn@grs.de

The safety against radioactive waste stored deeply in the underground is principally at risk where groundwater can attack the metallic waste canisters. For a performance assess-ment of a geological repository, it is therefore imperative to know the groundwater flow system over the projected lifetime of the repository. According to the current legislation in Germany, this will be a million years /STA 17/.
Over the past million years, several cold ages have occurred and have brought permafrost conditions basically to all potential sites for a radioactive waste repository in Germany (e.g. /VAN 93/). It can therefore be expected quite safely that any conceivable repository will sooner or later be subject to these conditions again. This is significant because permafrost will have a considerable impact on groundwater flow as the ground freezing tends to sepa-rate aquifers in the underground hydraulically from the surface.
However, it is also known that even under permafrost conditions there are local volumes of unfrozen ground, called taliki, connecting the surface waters with unfrozen aquifers. Flow of contaminated waters from a possible leakage in the repository could thus be directed towards such taliki and reach the surface concentrated in single spots (e.g. /JOH 16/). Taliki are thus a key feature in the assessment of a possible exposure of the biosphere to harmful radioactive substances.
Talik formation is presently quite intensively investigated in the framework of global warm-ing and thereby refers to melting processes (e.g. /PAR 18/). In case of geological storage of radioactive waste, by contrast, the question is rather, where open taliki will remain in an otherwise increasingly freezing ground. Taliki are not accessible to direct observation even though they can be detected by laborious field work. Insight into the processes of talik formation might therefore alternatively be gained by numerical modelling.
A surprisingly large variety of mathematical formulations can be found in the literature that describe groundwater flow under freezing conditions including ice formation and may be applied to the problem at hand. To ensure that all relevant processes are appropriately addressed in an own model of choice, though, general balance equations for groundwater and heat flow are developed from scratch without prematurely introducing assumptions and restrictions. These balance equations are supplemented by constitutive equations and equations of state (EOS) covering also sub-zero temperature conditions. Additionally, a computationally less demanding set of EOS valid in the temperature range between 20℃ and +60℃ and hydraulic pressure up to 20 MPa has been developed. The ensuing math-ematical model is then numerically realised in the framework of the code COMSOL Mul-tiphysics.
For realistic boundary conditions at the model surface, the air temperature evolution over the last 400,000 years determined from ice cores from Antarctica /JOU 07/ has been adapted to the location of present Germany. Heat flux from inner earth can be shown to be approx-imately constant over this time period of time. First results from modelling ground temperatures during the beginning of an ice age confirm a thermal shadowing of the cooling ground under large aquatic surface features.

Participation:

In-Person

References:

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Supplement to: Jouzel, J., Masson-Delmotte, V., Cattani, O., Dreyfus, G., Fa-lourd, S., Hoffmann, G., Minster, B., Nouet, J., Barnola, J.-M., Chappellaz, J.A., Fischer, H., Gallet, J.C., Johnsen, S.J., Leuenberger, M.C., Loulergue, L., Luethi, D., Oerter, H., Parrenin, F., Raisbeck, G.M., Raynaud, D., Schilt, A., Schwander, J., Selmo, E., Souchez, R.A., Spahni, R., Stauffer, B., Stef-fensen, J.Peder., Stenni, B., Stocker, T.F., Tison, J.-L., Werner, M., Wolff, E.W.: Orbital and millennial Antarctic climate variability over the past 800,000 years. Science, 317(5839), 793-797, 2007, https://doi.org/10.1126/science.1141038
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Energy Transition Focused Abstracts:

Poster / 501

Investigating interfacial instability snap-off in a uniform capillary with a sharp wettability contrast

Authors: Yemna Qaiser[1]; Harris Rabbani[1]; Thomas Seers[1]; Talha Khan[1]

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Understanding two-phase flow in porous media is highly significant in many fields of science and engineering in terms of both theory and practice. Fundamentally, pore-scale immiscible displacement is governed by the wettability of the pore-wall, which in turn, influences the distribution and transport of the fluid phases at the micro- to macro-scale. Whilst two-phase transport mechanisms in strongly-wetting and weakly-wetting systems are well described, there is a general lack of understanding of the fluid invasion protocol in mixed-wet regimes 1, as spatial heterogeneity in surface wettability gives rise to additional complexity in terms of the governing physics of the immiscible fluid flow. Snap-off is a major pore-scale immiscible fluid transport and immobilization mechanism which occurs during imbibition, which causes the entrapment of the non-wetting phase owing to the presence of strong interfacial forces. It is governed by pore geometry and pore surface wettability. Indeed, it is important to recognize the relative influences of each of these factors when attempting to characterize such instabilities. Most research conducted hitherto has studied snap-off under mono-wet conditions; the work of Zhao et al., however, sheds the light on the understanding of snap-off in partial wetting conditions [2]. In addition to these systems, many naturally occurring pore networks exhibit sharp wettability contrasts across their pore walls (e.g. wettability altered mixed-wet carbonate reservoirs). In this work, we propose that such wettability contrasts can give rise to fluid interfacial instabilities capable of producing snap-off-like behavior (i.e. droplet formation) within pore-systems exhibiting invariant geometry (i.e. straight capillary tubes).
To investigate the behavior alluded to above, we perform high-speed microfluidic experiments and complimentary computational fluid dynamics (CFD) simulations. Microfluidic experiments are conducted within uniform (circular) capillaries with a sharp wettability contrast perpendicular to the flow axis, whereby the inlet side of the capillary is superhydrophobic and the outlet portion is hydrophilic. By injecting deionized water into the air saturated capillary, we are able to record the occurrence of a novel instability, whereby the injected fluid phase dislocates at the juncture between the aforementioned wetting regimes. Additionally, finite volume CFD simulations have been performed to probe the nature of this novel interfacial instability over a range of capillary numbers and wettability contrasts. Our results demonstrate that for strong wettability contrasts at low displacement rates (i.e., low capillary numbers), as the interface reaches the boundary between the two distinct wetting regimes, it elongates, enhancing meniscus curvature, which eventually leads to snap-off of the injected fluid phase. This phenomenon has wide-reaching implications towards numerous fields, such as those concerned with bio-fluid dynamics, hydrocarbon recovery, and CO2 sequestration, as well as potential applications within microfluidics / lab-on-chip diagnostics, providing the ability to generate droplets using sharp wettability contrasts in lieu of constrictions in pore or channel geometry.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 502

Micromodel porous network with heterogeneous wettability

Authors: Camille BRIGODIOT[1]; Elliot SPEIRS[1]; Nicolas PANNACCI[1]; Cedric GUYON[2]; Michael TATOULIAN[2]

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Micromodels are 2D transparent model porous networks allowing for observations and quantification of numerous phenomena involved in fluid flow in porous media. In the context of energy studies, such as for CO2 storage or geothermal energy, micromodels are increasingly used. At the pore scale considered (i.e., roughly 10 - 100 µm for the micromodel), effects of surface and interfacial properties are enhanced when compared to larger scales. From an experimental point of view, being able to control wettability is thus crucial to gain in representativeness of micromodels so as to better understand diphasic and multiphasic flows in porous media.

This study focuses on the development of polymer micromodels with an increase of representativity by means of a spatially heterogeneous wettability obtained from localised silica coatings. Manufacturing involves photoetching, hot embossing of a COC polymer material (Cyclic Olefin Copolymer), localised deposition of a thin layer of silica (SiO2) by plasma polymerisation of TEOS (Tetraethyl orthosilicate) and closure of the micropattern by lamination. The surface treatment allows for a decrease in wetting angle from 87° (drop of water in air on untreated COC) to 30° (on treated COC). These steps have been optimised and the analyses show the stability of the surface treatment over several weeks. The model porous devices developed are designed for atmospheric pressure and ambient temperature working conditions. The resulting micromodels are used to show the influence of wettability heterogeneities on single and multiphase flows in a porous medium through several experiments, including the injection of a water-in-oil emulsion**.

** See also presentation "Tortuosity-governed droplet transport in a microfluidic porous network" (Elliot SPEIRS, Nicolas PANNACCI, Marie-Caroline JULLIEN, Maxime MOREAUD)

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 503

Modeling Structural Changes in a Fixed Bed Reactor for Thermochemical Heat Storage During Continuous Cycling

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As countries around the world are trying to transition away from fossil fuels to renewable energy sources, short- and long-term storage of an increasing, yet unsteady, renewable energy supply becomes a major challenge. Further, as provision of heat is a major part of industrialized countries' energy needs, storing heat energy, in applications such as the capturing of excess heat from industrial processes or concentrated solar power plants, has the potential for great increase in energy efficiency.
Among the available heat storage technologies, thermochemical heat storage provides a large energy capacity for short- and long-term storage. To further develop the technology, DLR is developing models and simulations as well as experimental characterization methods for thermochemical heat storage. More specifically, storage in the CaO/Ca(OH)2-System is investigated because of the low price and environmental friendliness of the reactants.
However, a major challenge to modelling such systems, is the restructuring of the powder bed during repeated cycling, i.e., repeated charging and discharging of the reactor. This happens through mechanical and chemical alteration of the powder bed. The three dominant effects are, the compaction of the bed from the gas flow, the expansion/shrinkage of the powder particles through water uptake/release and the agglomeration of powder particles, where bonds between the particles form, solidifying the bed.
To model the compaction and solidification of the powder bed during cycling, we present an elastoplastic mechanical model based on the Drucker-Prager-Cap yield surface, which has been used previously for powder compaction, see e.g. 1. The changes in the powder bed during cycling are modeled by hardening mechanisms, i.e., a changing yield surface, corresponding to powder compaction and agglomeration, respectively. While the exact mechanism of the agglomeration is yet unknown, it can be characterized by mechanical measurements.
Then, the plastic model is coupled to a reactor model, simulating the heat and mass transport, as well as the thermochemical reaction using a model, similar to [2]. This enables the study of the powder bed dynamics under different boundary conditions during cycling, such as pressure drop, water vapor fraction and reactor geometry.
In this contribution, we will present a parameterization of the model based on experimental data, that was obtained from a test reactor, and the parameterization of the mechanical model, i.e. the plastic yield surface, is done via flow tester experiments.
Then, we will show simulation results with an emphasis on investigating the irreversible effects of continuous cycling on the powder bed. This includes the compaction of the powder bed during the pressurization of the reactor, the possible emergence of hysteresis effects in the deformation of the powder bed under repeated cycling, as well as degradation through irreversible structural changes, such as powder agglomeration.

Participation:

In-Person

References:

1 Wu, C.-Y & Ruddy, O.M. & Bentham, A.C. & Hancock, B.C. & Best, Serena & Elliott, James. (2005). Modelling the mechanical behaviour of pharmaceutical powders during compaction. Powder Technology. 152. 107-117. 10.1016/j.powtec.2005.01.010.
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Part 1 –Conceptual model. Energy. -. 10.1016/j.energy.2013.06.025.

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MS06-B / 504

Direct nanoscale investigation of calcite dissolution kinetics

Authors: Chiara Recalcati[None]; Martina Siena[1]; Monica Riva[1]; Alberto Guadagnini[1]

[1] *Politecnico di Milano*

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We illustrate experimental protocols designed to acquire Atomic Force Microscopy (AFM) images for the nanoscale investigation of key patterns of mineral dissolution reactions at solid-fluid interfaces. These reactive processes are critical in numerous scenarios of application in natural porous systems as they drive alterations of fundamental properties of the host solid matrix (e.g., permeability, porosity, and storage capacity). Advanced high resolution imaging techniques such as the AFM or the Vertical Scanning Interferometry (VSI) enable direct observation of crystal surfaces subject to reaction and document the presence of several local processes that contribute to the space-time development of the reaction. The action of these processes, in turn, yields marked spatial heterogeneities in the strength of reaction rates even at such very small scales, thus hampering the possibility to exhaustively represent material flux across the crystal surface through an average rate value. In this framework, a stochastic characterization of the reaction kinetics is then important to account for such spatial variability. We consider different setups designed to mimic conditions that are typical of natural scenarios of environmental concern, such as (i) diffusion-dominated and (ii) surface-controlled conditions. The former are typical of (extremely) low velocity/stagnant regions (e.g., dead-end pores), whereas the latter resemble flowing areas. We show through qualitative and quantitative analyses that data obtained via the proposed experimental settings can be readily employed for the evaluation of reaction rate maps that are then well suited for interpretations grounded on stochastic characterization approaches.

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MS01 / **505**

Injectivity losses in sandstones during CO2 hydrates formation

Author: Matthieu Mascle[1]

Co-authors: Ameline Oisel [1]; Nicolas Gland [1]; Anne Sinquin ; Raymond Jellema [2]; Luc Pauget [2]; Souhail Youssef

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Sequestration of captured CO2 in geological formations to reduce its content in the atmosphere is one proposed solution to mitigate global warming. This solution, generally referred as carbon geo-sequestration (CGS), involves the injection of CO2 into depleted reservoir or saline aquifers. The success of CGS relies on many technical aspects, including CO2 plumes extension, gravity segregation, capillary trapping, and well's injectivity. Well's injectivity, which refers to the ability of the injected CO2 to flow near the wellbore zone, is crucial in the design of CGS operation as it constrains the maximum flow rate at the well. In the case of depleted reservoir, pressure of the reservoir can be as low as 20 bars. In the other hand, to fulfill a minimum volume flow rate, CO2 is injected with pressure higher than 50 bars. This pressure difference near the well bore causes the CO2 to undergo both a considerable adiabatic depletion and a phase transition, reducing the temperature of the fluids and the rock. The co-existence of both CO2 and brine, at relatively high pressure and low temperature may bring the system in hydrates stability zone and led to a CO2 hydrates formation. This crystallization can increase the volume of immobile phases in the pore-space. Consequently, the relative permeability of the rock to CO2 can be drastically reduce. In the worst scenario this can lead to the complete clogging of the injection wells.
The formation of CO2 hydrates in partially saturated porous media has been widely investigated at local scale using high resolution micro-computed tomography (micro-CT). To a lesser extent, the reduction of CO2 injectivity has been explored under flowing conditions in coreflooding devices. The purpose of this work is to trigger and observe the formation of CO2 hydrates in sandstones under flowing conditions, and to evaluate the loss of CO2 injectivity during the crystallization process as a function of initial water saturation. Experiments have been conducted using a high throughput experimentation setup (CAL-X 1) equipped with a coreflooding device allowing running experiments on small rock plugs, with respectively length and diameter of 2 cm and 1 cm. It uses X-ray to live-monitor changes in fluids saturation. Experiments of hydrate formation have been conducted at 25 bars and 5℃, for different initial brine saturations, and on various rock-types, targeting different porosities, permeabilities and clay content. Relative permeabilities curves accounting for the formation of CO2 hydrates in the porous media were interpreted from those experiments.

1 Youssef, S., Mascle, M., and Vizika, O., 2018, High Throughput Coreflood Experimentation as a Tool for EOR Project Design, Paper SPE-190166 presented at the SPE Improved Oil Recovery Conference, Tulsa, Oklahoma, USA, 14–18 April. DOI: 10.2118/190166-MS

Participation:

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506

Solute and Particle Transport into thin Porous Media: from Microfluid Perspective

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Latex particles are used in the inkjet printing industry to improve printing quality. Although the end state of the particle transport has been investigated extensively, limited do we know about the dynamic process due to its small spatial scale and short temporal scale within the thin porous media. Thanks to the advance in microfluidic fabrication, we are able to combine fluorescence microscopy and fluorescence recovery after photobleaching (FRAP) techniques with microfluidic experiments for direct observation on the dynamic process of particle and solute transport into thin porous media in a magnified scale. The experimental observation complies with phenomena seen in real paper substrates and theoretical predictions of the extended DLVO theory revealing the impact of particle clogging, hydrophobicity alteration.

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Poster / 507

Solute transport in partially saturated porous media with spatially correlated disorder

Authors: Ali Saeibehrouzi[1]; Ran Holtzman[2]; Petr Denissenko[3]; Soroush Abolfathi[3]

[1] *University of Warwick & Coventry University*

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Solute transport in porous materials is important in many natural and industrial applications, such as soil contamination and subsurface CO2 storage. While in many cases there is more than one fluid phase (”partially unsaturated” conditions), most studies focus on the simpler case of the single-fluid phase (”saturated”). This study investigates the effect of spatial correlations in pore sizes on fast two-phase displacement under an unfavorable viscosity ratio (viscous fingering regime), using Direct Numerical Simulation (DNS). We consider immiscible fluids and simulate transport in the invading (lower viscosity) fluid phase. Considering the short timescale of invasion compared to that of solute transport, for computational efficiency and avoiding the transient velocity streamlines affecting transport, the latter is simulated only once the fluid phase distribution reaches steady-state. Analysis of the developed DNS model shows that spatial correlation affects solute transport via the distribution of mobile and trapped regions. The Probability Density Function (PDF) of pore-scale Peclet number shows a bimodal variation with (1) highly advective and (2) highly diffusive regions. While for the saturated case transport is mainly controlled by advection, the creation of stagnant zones in the partially-saturated case focuses the solute into narrow regions. The numerical results show that the inclusion of a second fluid phase increases dispersivity, and reduces breakthrough time with a sharp gradient of solute concentration between stagnant and flowing regions.

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In-Person

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Energy Transition Focused Abstracts:

MS07 / 508

Investigations of Degenerate Equations for Fluid Flow and Reactive Transport in Clogging Porous Media

Authors: Nadja Ray[1]; Simon Zech[1]; Raphael Schulz[1]

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Structural changes of the pore space and clogging phenomena are inherent to many porous media applications. However, related mathematical investigations remain challenging due to the degeneration of the hydrodynamic parameters. In this research, we apply an appropriate scaling of the unknowns and work with porosity-weighted function spaces. This enables us to prove solvability of a coupled flow and transport problem with degenerating, but prescribed porosity field, permeability and diffusion tensor. Moreover, we conduct numerical simulations for the combined, degenerating flow and transport problem. As discretization method, lowest order mixed finite elements are used and stability of the numerical scheme is shown. Under certain additional regularity assumptions, convergence (with optimal order) can be proven. Our numerical results confirm that optimal convergence is obtained for the transformed variables whereas the non-transformed variables might not converge.

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Energy Transition Focused Abstracts:

MS01 / 509

Effect of rock heterogeneity on pore-scale fluid displacement in a layered sandstone for underground hydrogen storage

Authors: Zaid Jangda[1]; Hannah Menke[1]; Andreas Busch[1]; Sebastian Geiger[None]; Tom Bultreys[2]; Kamaljit Singh[1]

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[2] *Ghent University*

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A safe and efficient hydrogen storage mechanism will be crucial for the successful transition towards a green hydrogen economy. Underground storage of hydrogen can be a viable option for short to long-term storage to meet the fluctuations in energy demand. However, there is limited understanding of the pore-scale displacement and trapping mechanisms for hydrogen-brine systems, especially in heterogeneous rocks at reservoir conditions. Our recent experimental study 1 allowed us to understand the trapping of hydrogen within the pore space of a homogeneous sandstone rock and showed dissolution of hydrogen in the resident brine after injection and production of hydrogen at subsurface conditions. In this work, we build on these findings and use X-ray micro-tomography to study the pore-scale fluid displacement processes during cyclic injection of hydrogen in a layered sandstone rock sample. We investigate how the presence of a thin and low permeability layer between two high permeability zones in the rock sample affects fluid displacement processes and hydrogen trapping. The results indicate that hydrogen preferentially occupies the higher permeability zones, and the residual hydrogen saturation increases in subsequent cycles. The findings from

this experiment contribute towards the selection of the most suitable subsurface formations for underground hydrogen storage. Extending our research to perform time-resolved synchrotron X-ray imaging experiments will provide additional insights into the dynamics of pore-scale processes in layered reservoirs during underground hydrogen storage.

Participation:

In-Person

References:

1 Jangda et al., 'Pore-scale visualization of hydrogen storage in a sandstone at subsurface pressure and temperature conditions: Trapping, dissolution and wettability', Journal of Colloid and Interface Science, vol. 629, pp. 316–325, Jan. 2023, doi: 10.1016/j.jcis.2022.09.082.

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MS06-B / 510

The traveling wavefront for foam flow in multi-layer porous media

Authors: Grigori Chapiro[1]; Luis Fernando Lozano Guerrero[2]; Andrés Castrillón Vásquez[3]; Jhuan Cedro[3]; Weslley da Silva Pereira[4]

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The injection of foams into porous media has gained importance as a method of controlling gas mobility. The multilayer structure of the porous medium raises a question about its efficiency in dealing with layers of different permeabilities. The present work shows the existence of a single traveling wavefront in a two-layer porous medium for a simplified model derived from a realistic two-dimensional one. Besides the necessary conditions for the solution's existence, we prove that the traveling wave velocity is a weighted average of the velocities as if both layers were isolated. All theoretical estimates were validated through one- and two-dimensional simulations. Finally, we estimated the order of magnitude of the characteristic time the traveling wavefront needs to stabilize.

Participation:

In-Person

References:

The traveling wavefront for foam flow in two-layer porous media
A.J. Vásquez, L.F. Lozano, W.S. Pereira, J.B. Cedro, G. Chapiro
Computational Geosciences 26 (6), 1549-1561, 2022

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MS22 / 511

Interaction of bubble dynamics and manufactured porous electrodes in flow through membraneless water electrolysis

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Co-author: Mohamed Mamlouk [1]

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Low cost hydrogen production is essential to meet global hydrogen production targets by 2050. Therefore research into alternative water electrolysis device design may lead to reduction in capital costs. One emerging alternative to the capital cost is the use of membraneless electrolysers. In particular we focus on diverging flow through membraneless devices which utilise cell and porous electrode geometry to separate hydrogen and oxygen without a separator or membrane. They can also utilise alkaline conditions allowing for lower cost catalyst and construction materials.

However, the technology is not commercial and the influence of the design of the device and the manufactured porous electrode properties are unknown. Computational fluid dynamic simulations (OpenFOAM) using the volume of fluid method is used to model the two-phase flow of hydrogen and oxygen bubbles coupled to electrochemistry. Different device geometry, porous electrodes, flow and current density are varied to investigate their impact on the cell potential.

Electrolyte flow distribution and scaling of the devices are investigated, which are highly dependant on the sizes of the pores, electrode gaps and higher Reynolds number flows. The initial results show that there is an interplay between the pore size and the electrode length in order to maintain uniform flow across the electrode, which is important to reduce bubble blockage of the electrode surfaces. The effect of the electrode microstructure on the current density distribution are evaluated and strategies to avoid bubble accumulation are discussed. Changes to the porous electrode morphology through advanced manufacturing techniques, along with the wettability and device flow geometry could lead to higher efficiency, low capital cost water electrolysis.

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512

The influence of pore-body-to-pore-throat aspect ratio on emulsification

Authors: Ahmad Kharrat[1]; Judy Jalkh[None]; Holger Ott[1]

[1] *Montanuniversität Leoben*

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The structure of the porous media may be an important factor to be considered in designing effective displacement agents for tertiary oil recovery and soil remediation. Rock properties such as pore-body-to-pore-throat aspect ratio, coordination number, and pore-size distributions are known to impact multiphase flow in porous media. In addition, pore geometry can affect emulsion sizes and their stability in the presence of an emulsion phase. The present study deals with the immiscible and near-miscible fluid displacement under different flow regimes and in pore systems with well-defined geometrical properties.

In order to investigate the influence of rock properties, we developed a lab-on-a-chip approach based on optical and fluorescence microscopy. With this approach, we are able to decompose rock structures with respect to classical petrophysical parameters. In this study, we focused on the pore-body-to-pore-throat aspect ratio and pore-body distances and varied these properties in otherwise generic pore structures. In this frame, we designed and used several sets of glass made microfluidic. Distilled water and surfactant solution with different salt concentrations as the aqueous phase and decane as the oleic phase were used during these experiments. Different designs of pore structures next to several fluid compositions give us better insight into fluid displacement in pore scale.

We observed how aspect ratio impacts emulsion formation, its texture, and stability over time. We analyze the data on the basis of residual oil saturation, emulsion formation, and velocity calculation on the first contact and throughout the displacement process. By increasing the aspect ratio, we observed that the remaining oil saturation at first contact, front velocity, and emulsion stability are also increasing. Regardless of the aspect ratio, the emulsion formed at the first contact displacement happened in the out-of-optimum condition. Besides, lower trapped oil was observed by increasing the distance between pores.

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Energy Transition Focused Abstracts:

Poster / 513

Quantifying the Influence of Groundwater Flow on Bacterial Chemotaxis near a NAPL Contaminant Source at the Pore Scale

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[1] *University of Virginia*

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Bioremediation of nonaqueous phase liquid (or NAPL) contaminants may be accelerated with the presence of chemotactic bacteria that can preferentially migrate toward NAPL upon detecting its chemical gradient. In a heterogeneous porous media 1, chemotactic bacteria accumulated in dead-end pores near NAPL ganglia trapped in low-permeable regions; however, no retention was seen in bacteria near NAPL surfaces distributed in the high-permeability area or along preferential flow pathways. Groundwater flow is a critical feature of contaminated sites in the subsurface and its influence on bacterial transport and chemotaxis remains a challenging aspect to predict.

In this work, we investigated the impact of fluid velocity on chemotactic response at the pore scale using a combination of microfluidic experimentation and continuum modeling. A bacterial suspension flowed parallel to a flat NAPL-water interface over a range of typical groundwater flow rates (0.5-10 m/d) in a T-shaped microfluidic device. In chemotaxis experiments, the side capillary in the T-shaped channel (50 μm in opening) was filled by a NAPL mixture containing chemoattractant naphthalene. Soil bacteria *Pseudomonas putida* G7 (PpG7), chemotactic to naphthalene, were introduced in the main microchannel. At a fluid velocity of 0.5 m/d, greater densities of PpG7 were seen in the vicinity of the NAPL-water interface. As flow velocity increased to 10 m/d, we observed near the interface reductions in bacterial density and residential area (*i.e.*, where normalized bacteria density >1).

In continuum modeling, bacterial transport was described by a modified diffusion-convection equation. The diffusion coefficient (Db) represented uniform spreading in a bacterial population due to motility. For chemotactic bacteria, a chemotactic velocity as a function of chemical concentrations and bacterial intrinsic properties (*e.g.*, chemotactic sensitivity coefficient χ_o), was added to convection to account for biased migration toward the NAPL source. Simulations indicated that chemotaxis was suppressed in flow as diffusion and sensitivity coefficients (Db, χ_o) were both reduced to different extents as fluid velocity increased. Bacteria near the NAPL surface experienced shear stress, which might interfere with reorientations in bacterial trajectories so that their swimming became more aligned with flow direction in higher flow velocities [2]. Therefore, reductions in bacterial retention near the NAPL-water interface might stem from the modifications in cell motility due to shear. Bacteria in contaminated subsurface environments are often subject to groundwater flow whose influence on bacterial transport is vital for the implementation of bioremediation. This work revealed that bacterial chemotaxis in shear flow was hampered to a greater extent than predicted by convection. Findings from this study can aid in assessing the significance of chemotaxis in cell navigation of contaminated subsurface aquifers.

Participation:

In-Person

References:

1 Gao B, Wang X, Ford RM. Chemotaxis along local chemical gradients enhanced bacteria dispersion and PAH bioavailability in a heterogenous porous medium. Sci Total Environ. 2023 Feb 10;859(Pt 1):160004. doi: 10.1016/j.scitotenv.2022.160004. Epub 2022 Nov 8. PMID: 36368405.

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Energy Transition Focused Abstracts:

MS01 / **514**

Experimental measurements on caprock CO₂-water wettability at reservoir pressure and temperature

Authors: Mohamed M. Awad[1]; D. Nicolas Espinoza[1]

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Most CO₂ geological storage sites, such as saline formations and depleted hydrocarbon reservoirs, rely on structural trapping provided by the caprock and fault gouge material as one of the trapping mechanisms. Clay- and quartz-rich caprocks are expected to be water-wet at reservoir conditions and create a positive capillary pressure to ensure CO₂ trapping. However, most experimental studies so far have limited to either temperature lower than 60℃ or pressure lower than 25 MPa posing uncertainties about high-temperature and high-pressure conditions. This study shows the result of water imbibition experiments in synthetic caprock at temperature equal or larger than 60℃ and pressure equal or larger than 25 MPa. The results show spontaneous imbibition of water droplets in synthetic caprock partially saturated with supercritical CO₂ and water. Thus, the results show that caprock building minerals remain water-wet to CO₂ at typical temperature and pressure reservoir conditions. The results indicate that clay- and quartz-rich caprock and fault gouge are expected to develop a positive entry and breakthrough pressure (i.e., P_{CO2} - P_w > 0 MPa), thus, favoring CO₂ structural trapping.

Participation:

In-Person

References:

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Poster / 515

Employing GPUs to compute effective properties of porous media from µCT scans in desktop computers

Author: Pedro Cortez Lopes[1]

Co-authors: André Pereira [1]; Ricardo Leiderman [1]

[1] *Universidade Federal Fluminense*

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Image acquisition techniques are increasingly being employed for material characterization. For example, X-ray Mirco-Computed Tomography (μCT) can be seen in multiple works that study media such as reservoir rocks [2,3], and fibrous and woven materials [4,5], to cite a few. This sort of approach usually involves 3D numerical simulations at the microstructure, which is represented as a grid of voxels, to compute the effective properties of the sample. For μCT scans, these simulations can be significantly large and with high memory allocation, to the point that clusters or even supercomputers might be required. One of the ways to perform these simulations is via the voxel-based Finite Element Method (FEM), where each voxel is taken as an element, thus eliminating the task of meshing the domain, and favouring the adoption of lightweight matrix-free schemes. We have been exploring memory-efficient implementations of such method for Numerical Homogenization, as it can be seen in 1, where massively parallel (GPU) solvers are detailed for thermal conductivity and elasticity analyses. We have also recently implemented solvers for other phenomena, such as Stokes flow in porous media, to compute permeability. The motif in these implementations is not storing data that can be recomputed on demand, and tackling the trade-off in computational cost with acceleration provided by graphics cards. Here, we aim to present how our solvers can be used to characterize segmented μCT samples with personal hardware in a sensible time frame. Image-based meshes with hundreds of millions of voxels can be studied with less than 8 GB, taking seconds or no more than a few minutes per simulation. This enables analyses on μCT images with upwards of 400^3 voxels in desktop computers equipped with relatively accessible GPUs. It will be shown that even a personal laptop can be used for thermal conductivity or electrical resistivity analyses of such dimensions. Further, a case-study in the context of Digital Petrophysics will be presented, where the electrical resistivity, linear elastic stiffness, and absolute permeability of sandstone μCT samples are computed employing our tools and methods, in workstations equipped with a single GPU, of either 8 or 12 GB RAM. These analyses would not be feasible with such limited memory allocation if not for the matrix-free approach, nor would they take minutes if not for the massively parallel solver.

Participation:

In-Person

References:

1 Lopes, P. C. F., Pereira, A. M. B., Clua, E. W. G., and Leiderman, R. (2022). A GPU implementation of the PCG method for large-scale image-based finite element analysis in heterogeneous periodic media. Computer Methods in Applied Mechanics and Engineering, 399:115276.

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MS05 / **516**

Bacterial Accumulation near Residual Organic Pollutants in Micropockets of Porous Media Depends on Chemotaxis and Pore Water Velocity

Authors: Beibei Gao[1]; Roseanne Ford[None]

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Groundwater contamination caused by nonaqueous phase liquids (NAPLs) is a significant environmental concern as NAPLs are ubiquitous and persistent pollutants, remaining recalcitrant to bioremediation due to their low solubility and limited bioavailability. Chemotaxis, the biased migration of motile bacteria toward chemical gradients, may facilitate remediation of NAPLs by transporting pollutant-degrading bacteria to residual contaminant sources trapped within the soil matrix. Greater accumulation of chemotactic bacteria was observed in Gao and coworkers'study near NAPL contaminants at the juncture between different permeability regions in a heterogeneous micromodel 1. Bacterial distributions in the pore space were influenced by chemical gradients and fluid flow, whose combined effect on bacterial transport is not well characterized in porous media. In this work, we aimed to investigate the transport mechanism of chemotactic bacteria from moving pore water into stagnant micropockets formed by oil-phase contaminant ganglia.
Chemotactic bacteria (*Pseudomonas putida* G7) were introduced at varying fluid flow rates (0.2-56 m/d) into a dual-permeability microfluidic device contaminated by NAPL. Bacterial suspension flowed preferentially through the highly permeable area while the low-permeability regions retained NAPL, which served as contaminant sources. Bacteria showed accumulation in micropockets near junctures of high- and low-permeability zones due to chemotaxis. However, accumulation in micropockets was initially increased and then decreased as pore fluid velocity increased in each trial. Convection in porous media did not simply override chemotaxis as previously observed in bulk liquid [2]; instead, higher pore velocity brought bacteria closer to NAPL sources than diffusion alone and triggered stronger chemotactic response by creating steeper chemical gradients. The optimal pore velocity, in terms of maximum bacterial accumulation, depended on the time scale of exposure to chemicals. Bacterial exposure time to chemical gradients was estimated to be $\tau e = L/Vp$, where L was characterize pore dimension and Vp fluid velocity. When exposure time exceeded response time (~ 2 s in Pseudomonas putida [3]), bacteria in bulk flow did not have sufficient time to bias their swimming directions in response to the presence of NAPL contaminants. Our results indicated that in heterogeneous porous media chemotaxis could be enhanced by fluid flow rather than merely being suppressed and chemotactic bacteria would lose their advantage when their exposure time to chemicals was below the threshold of response time.

Results from this study suggest that accumulation of NAPL-degrading bacteria in porous media micropockets will facilitate biofilm formation and enhance bioremediation. The dimensionless group of parameters comparing response time to exposure time will aid practitioners in determining an appropriate pore water velocity to use in delivering chemotactic bacteria for in situ bioremediation.

Participation:

In-Person

References:

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MS06-A / 517

Trapping Behavior of Gases from 4D Pore Scale Imaging

Authors: Ying Gao[1]; Tibi Sorop[1]; Niels Brussee[1]; Hilbert van der Linde[1]; Karin de Borst[1]; Rouhi Farajzadeh[1]; Steffen Berg[1]

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The trapping behavior of gases in porous rock plays an important role in many subsurface processes such as underground storage of carbon dioxide and hydrogen, and the production of hydrocarbons. Over the last decade several laboratory studies have demonstrated that the trapping behavior of gas can be different than that of an immiscible liquid [1-7]. It is challenging to experimentally measure the trapped gas saturation (Sgr) in the laboratory, as the gas compressibility, partitioning/solubility and diffusion effects largely impact the spatial evolution of fluid and gas phases. The uncertainty in Sgr is often so large that it could have significant impact on field development decisions. Experiments with 3D pore scale imaging have already revealed details of physicochemical processes. In the particular case of trapped gas saturation, it is furthermore important to develop a more general understanding of gas dynamics at the pore scale, i.e. an understanding of dynamic processes, which requires then 4D imaging (3D + time).

The pre-equilibration of liquids e.g. brine with gas is necessary to measure Sgr [6]. However, it has been observed that trapped gas still dissolves over time –the mechanism of which is not fully understood yet [1, 6]. Here, we present a 4D high resolution X-ray CT imaging technique in a study covering the effective in-situ behavior of a range of gases, including compressed air, CH4 and H2,

inside the porous media. Using a novel laboratory-based micro-CT scanner it was possible to acquire dynamic 3D images with high time resolution, which allows us to capture the intrinsic time scales of the gas dynamics.

The experiments confirmed the previous findings of a continuously decreasing gas saturation with more equilibrated brine injected, which even continued after the brine injection was stopped, resulting in very low (near zero) Sgr values 1. We find systematic differences between the gases studied. We divided the observed dynamics in two different regimes, the capillary trapping regime where the gas pathways from inlet to outlet are disconnected by snap-off, and the dissolution regime. We found more capillary trapping and also faster dissolution for CH4 and H2 than for compressed air.

From previous studies, based on pore scale occupancy and the relevance of diffusive transport [4, 5], Ostwald ripening is playing an important role, impacting the gas dynamic behavior. In this work, we found more supporting evidence for this interpretation. The dissolution time scale follows a trend that can be captured in the product of diffusion coefficient and gas solubility in the liquid measured by Henry law constant.

Participation:

In-Person

References:

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MS03 / **518**

Multicontinuum non-equilibrium theory for coupled flow and deformation in fractured rocks

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Coupled flow and deformation in fractured media is often modeled by the classical dual-porosity poroelasticity theory. The latter is based on the Barenblatt hypothesis of pressure equilibrium inside the rock matrix. This is a reasonable assumption if the characteristic time scales for pressure propagation in the matrix are comparable or smaller than the characteristic fracture time scales. Under large permeability contrasts between the fracture and matrix domains, these conditions may not be met, and the flow and deformation behaviors are dominated by non-equilibrium effects, which manifest in long-tails in flux responses. Using volume averaging, we derive a multicontinuum approach that accounts for pressure non-equilibrium in the rock matrix, and compare it to the classial dual porosity approach. We use explicit analytical solutions to identify the dominant time scales and time regimes, and to evaluate the scaling behaviors of the flux response in consolidation and production scenarios. The flux evolution at a production well is characterized by decay behaviors that are different from the classical dual porosity approach. These behaviors are related in the proposed multicontinuum theory to the permeability contrast and the permeability distribution across the matrix blocks.

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MS07 / **519**

Chemo-Hydro-Mechanical variational phase-field fracture model in cementitious systems

Authors: Mostafa Mollaali[1]; Renchao Lu[1]; Vanessa Montoya[2]; Olaf Kolditz[1]; Keita Yoshioka[3]

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We present a fully coupled chemo-hydro-mechanical variational phase field model for simulating fracture initiation and propagation, including chemical reactions in cementitious systems. In a staggered approach, we coupled three subprocesses: (i) fluid flow in porous media, (ii) reactive transport, and (iii) mechanical deformation of fractured porous media using the variational phase field.

We use the geochemical package PHREEQC 1 coupled in an operator-splitting approach with a finite element transport solver to calculate chemical reactions in thermodynamic equilibrium (dissolution or precipitation) while taking into account changes in porosity. We couple mechanical deformation and fluid flow using the fixed-stress splitting approach. For chemical damage, we introduce a variable to a constitutive relation that represents a degree of chemical damage ranging from zero (intact) to one (damaged material). The chemical damage variable represents changes in porosity caused by chemical reactions independently from the phase field variable that represents the mechanical damage [2]. Additionally, as effective diffusion and hydraulic conductivity increase in the presence of fracture and changes in porosity, phase field variable, and chemical damage should impact the hydraulic conductivity [3] and the diffusion coefficient [2, 4, 5].

We conducted different benchmarks to demonstrate the model's capabilities and properties to capture the fracture initiation and propagation due to chemical reactions. The proposed model was implemented in the open-source finite element framework OpenGeoSys [6, 7]. The research work has been conducted in the frame of the EURAD project (in particular in the WP MAGIC).

Participation:

In-Person

References:

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MS03 / 520

The importance of understanding hydrothermal alteration in fault related geothermal systems in Cornwall

Authors: Nathaniel Forbes Inskip[1]; Nick Harpers[2]; Hannes Claes[3]; Sabine den Hartog[2]; Andreas Busch[2]

[1] *Heriot-Watt*

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Depending on the geographical and geological setting, geothermal energy is one of the few renewable energy sources that can supply a constant and reliable source of low-carbon heat and electricity. In the UK, the greatest potential for power generation from geothermal resources is limited to high-heat producing granites in SW England. It has long been known that there is the potential for geothermal energy extraction from Cornish granites. However, until recently, project development has been slow, with the United Downs Deep Geothermal Power (UDDGP) project being the first one to be developed in the UK. The UDDGP will operate on the principal of producing hot fluids (>170℃) from the Porthtowan Fault Zone (PFZ), which is hosted in the Carnmenellis Granite, at ~4.5km depth and re-injecting the fluids using a subsequent well intercepting the same fault zone at ~2.5km depth. Project viability is dependent on how much fluid is stored within the PFZ and surrounding rock mass (porosity), and the ability of fluid to flow through it (permeability).

Granite is considered a low porosity and permeability rock, where fluid flow through it is usually controlled by fractures. The presence of mineral veins, as well as hydrothermal alteration of the surrounding rock mass, is evidence that hot fluids have passed through the PFZ (and other similar fault zones in Cornwall) in the past. Although hydrothermal alteration is common, its importance in granite-hosted geothermal resources has received little attention to date. In this research, we aim to understand how hydrothermal alteration may affect the transport properties of the PFZ, by measuring the petrophysical properties of samples of unaltered and hydrothermally altered Carnmenellis Granite.

Samples were collected from a fault zone at Holman's test mine (a mine which is situated within the Carnmenellis granite), analogous to that of the PFZ. Porosity was measured using Nuclear Magnetic Resonance (NMR), and permeability was measured using a combination of steady state and unsteady state methods, on both intact and fractured material. All experiments were conducted at room temperature, and permeability experiments were conducted at confining pressures between 4 –34 MPa.

We found that the porosity of the hydrothermally altered material (10%) is much higher than that of the unaltered material (1%), and that the matrix permeability of the hydrothermally altered material is ~4 orders of magnitude higher than that of the unaltered material. However, the permeability of fractured hydrothermally altered samples is lower than that of fractured unaltered samples. We suggest that the results from the fractured samples is due to the altered material being weaker and more ductile than the unaltered material, and under confinement, asperities deform more, which leads to a reduced aperture and consequently permeability.

Our results demonstrate that the altered material has the potential to store significant amounts of hot fluid in the subsurface, and that there may be an important contribution from the matrix in terms of flow, outwith the fractures. Crucially, our results highlight the importance of fully characterising the reservoir so that accurate resource predictions can be made.

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MS09 / **521**

Pore-scale Ostwald ripening of residually trapped CO2 in the presence of oil and water at immiscible and near-miscible conditions

Authors: Deepak Singh[1]; Helmer Andrè Friis[1]; Espen Jettestuen[2]; Johan Olav Helland[2]

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Subsurface CO2 storage is a means to limit emissions to the atmosphere and global warming. Residual trapping, which occurs when brine invades the pore space occupied by the migrating CO2 plume and creates disconnected CO2 ganglia, is one of the mechanisms by which significant amounts of CO2 can be stored safely in the subsurface 1. Experiments on rock samples show that larger amounts of CO2 can be residually trapped in the presence of both oil and water [2], suggesting depleted hydrocarbon reservoirs are suitable sites for CO2 storage. However, reservoir conditions and fluid compositions vary widely, leading to different three-phase displacement mechanisms and residual trapping from miscible to immiscible conditions. Further, mass transfer between phases may change the amount of residually trapped CO2 over time.

A residually trapped gas-bubble distribution will undergo mass exchanges through Ostwald ripening. It is a process that leads to mass transfer from bubbles having a higher chemical potential to bubbles with a lower chemical potential. Our previous study on three-phase ripening [3] has highlighted that the ripening of gas bubbles in the presence of oil and water can lead to different residual gas volumes in the two liquids and different order of bubble loss during evolution. In this work, we will analyse the impact of partial gas miscibility on ripening evolution.

This study uses a chemical-potential difference and level-set based methodology [3-5] that calculates mass transfer between bubbles through diffusion paths in oil and water and across oil/water interfaces. We use the Peng-Robinson equation of state to calculate gas bubble fugacity at reservoir conditions. We perform simulations on different idealised 2D homogeneous and heterogeneous porous media. In the 2D heterogeneous medium, we simulate oil-water-gas-water invasion cycles to generate residual phase volumes. We also use 3D pore-space images of a water-wet sandstone to simulate Ostwald ripening in near-miscible conditions on residual three-phase fluid configurations with isolated oil and gas ganglia obtained after a water-alternate-gas invasion cycle. We quantified the evolution of pressure, volume, surface area, and the number of residual bubbles, for different initial fluid distributions and saturations.

Our results show that the gas-liquid interfacial tensions, gas-liquid contact angles, and oil-water capillary pressures determine the residual gas bubble sizes in each liquid phase. Specifically, we find that the equilibrium volume of bubbles in the oil phase, as well as the range of bubble volumes in oil and water, are smaller for near-miscible conditions than for immiscible conditions. This decrease is due to larger gas-liquid contact angles in the near-miscible case creating smaller gas bubble pressure differences and less mass transfer (and lower mass transfer rate) even though the ratio of gas-water to gas-oil interfacial tensions increases with partial miscibility. During fluid redistribution, we also identify cases where the bubble coarsening leads to capillary instabilities and three-phase double displacements (e.g., oil displaces a gas bubble that displaces water), which can lead to lower residual gas trapping.

Participation:

In-Person

References:

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Poster / 522

A method to measure adsorptive-poroelastic properties for nanoporous adsorbents

Authors: D. Nicolas Espinoza[1]; Alexander Neimark[2]; Stephan Braxmeier[3]; Gudrun Reichenauer[3]

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The characterization of adsorbents has been long established in material science. However, the interplay of adsorptive and mechanical response (such as induced strain and stress) at high pressure

and high stress is relatively new. The typical dilatometer test used in adsorption science is just one particular case of the full range of poroelastic response with varing fluid (pore) pressure and external total (or confining) stress. Here we show a general method to measure directly the adsorption stress developed by adsorbents in the presence of a non-zero effective stress consistent with the Biot theory for poroelastic solids. The method follows an extension of a procedure to measure the Biot coefficient for non-adsorptive materials. We show the application of the method for compacted activated carbon and synthetic monolithic porous carbon (carbon xerogel) in the presence of He, CH₄ and CO₂. Helium serves to measure the base poroelastic response in the absence of adsorption. The adsorbates, methane and carbon dioxide, help measure the adsorptive response. The method can be also extended to other adsorbents such as clays, zeolites and kerogen.

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MS08 / 524

Generating synthetic images of unsaturated porous media with a multiscale multipoint statistics approach to study transport in two-fluid-phase systems

Authors: Laurent Talon[1]; Emma Ollivier-Triquet[2]; Daniela Bauer[3]; Benjamin Braconnier[3]; Souhail YOUSSEF[3]; Véronique GERVAIS[3]

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Human activity influences largely the unsaturated vadose zone. Located above water tables, the vadose is impacted by pollution, typically from agriculture and industrial activities. Therefore, understanding contaminant transport in the vadose zone is crucial for water resources management. However, there is still a lack of comprehension on dispersion in unsaturated porous media, and the subject remains an active research topic. Classical models such as advection-diffusion equation often fails to predict the dispersion, notably because of the increased heterogeneity in the multiphase system. Particularly, the link between the nature of the multiphase flow, the phase configuration in the porous medium and the dispersion stays unclear. Notably, experimental techniques often struggle to gather significant number of data and to consider long time dispersion. Therefore, we propose a multiscale multipoint statistic algorithm (MPS) to generate porous media images at different saturation of immiscible fluids. Generated images are based on experimental observations of immiscible

multiphase flow air/water in a complex porous structure. To evaluate the representativeness of MPS generated images, we first analyze structural properties like the grains and air clusters size and geometry. These properties, compared to the experimental image's ones, show a good match. Then, flow and transport are computed using Lattice-Boltzmann simulation in both experimental and generated images for different saturation. The resulting velocity distribution and concentration profile are very comparable. Particularly, the variances of the concentration profiles are very well reproduced. These results shows that MPS algorithm are willing to capture and reproduce the main pore scale features that govern flow and transport in a complex porous media. Therefore, the MPS algorithm could be used to generate a large number of images based on experimental images to study transport in unsaturated porous media. Notably, it allows more statistical coherence that leads to a better understanding of the link between two-fluid phase configuration and transport. Furthermore, we generate larger images (in comparison to experimental data) which allow us to get more insight on long time dispersion.

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MS19 / **525**

AN EFFICIENT TIME DOMAIN IMAGE-BASED FINITE ELEMENT IMPLEMENTATION TO SIMULATE WAVE PROPAGATION IN POROUS MEDIA

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In this work, we present an efficient 2D/3D Finite Element implementation to simulate the propagation of elastic waves, in the time domain, in porous media. The input data for our solution are binary images, of which each voxel can be solid or pore. We consider regular structured meshes composed of cubic elements, compatible with the image-based approach. Our implementation takes advantage of this regularity for the integration over each element. In addition, we lump the mass matrix to make it diagonal and use an element-by-element technique so that we never have to assemble and store the global mass and stiffness matrices. This strategy aims to provide large-scale simulations with low memory consumption. We use the Leapfrog technique for temporal integration, an explicit technique whose main feature is to improve numerical stability. We tested the implementation in different scenarios, such as oblique propagation of wave beams and oblique incidence on solid/solid interfaces. Furthermore, we apply the implementation described here to calculate the effective wave velocities of rock samples from their microtomographic images. We compared the results with the Finite Element elastostatic analysis.

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MS23 / **527**

Ultrasonic Study of Water Adsorbed in Nanoporous Glasses

Authors: Jason Ogbebor[1]; John Valenza[2]; Peter Ravikovitch[3]; Ashoka Karunarathne[1]; Boris Gurevich[4]; Maxim Lebedev[5]; Alexei Khalizov[1]; Gennady Gor[6]

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Thermodynamic properties of fluids confined to nanopores differ from those observed in the bulk. To investigate the effect of nanoconfinement on compressibility of water, we measured water adsorption isotherm concurrently with compressional and shear ultrasonic velocities for two nanoporous glass samples. These measurements yield the longitudinal and shear moduli of the water-saturated nanoporous glass as a function of relative humidity and allow estimation of the bulk modulus of the confined water using the Gassmann theory. The modulus estimated from the experimental data is noticeably higher than that of bulk water at the same temperature and exhibits a linear dependence on the Laplace pressure derived from the relative humidity. Our findings obtained for water, which is a polar fluid, agree with previous experimental and numerical data reported for non-polar fluids, suggesting that irrespective of their structure, confined fluids are stiffer than bulk fluids. Accounting for fluid stiffening in nanopores may be important for accurate interpretation of wave propagation measurements in fluid-filled nanoporous media, including in petrophysics, catalysis, and other applications in process sensing.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS16 / 528

Insights into Water Cluster Instabilities in Gas Diffusion Layers of Polymer Electrolyte Fuel Cells

Author: Tim Dörenkamp[1]

Co-authors: Federica Marone [1]; Mayank Sabharwal [2]; Jens Eller [1]

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4D X-ray tomographic microscopy (XTM) offers the possibility to obtain detailed insights into the water removal process through gas diffusion layers (GDL) of polymer electrolyte fuel cells (PEFC) [1-4]. Recent work on droplet formation and detachment cycle [5, 6] has provided insights into the inter-action between a percolating water cluster feeding a droplet on the GDL surface and allowed the cal-culation of the capillary pressure in the water cluster via surface curvature analysis. The work of Mu-larzcyk et al. [6] was limited to the analysis of a single percolating water cluster using a small active area of 0.005 mm2. Here we extend the previous study by using a catalyst coated membrane with 8 small active areas (0.0625 mm2) thereby, allowing the analysis of the development of multiple perco-lating water clusters, in addition to increasing statistics [7].

An operando XTM cell was imaged at the TOMCAT beamline of the Swiss Light Source with a scan rate of 1 Hz for 180 s after a current jump from OCV to 1 A/cm2 at 30℃ cell temperature and 100 % relative humidity of anode and cathode feed gases. In total 11 water breakthrough points were identi-fied that percolated from the 8 isolated active areas through a Toray TGP-H-060 GDL (10 %wt PTFE). This presentation will discuss the percolation process of individual water clusters with respect to their through-plane and in-plane growth to identify correlations between the water volume, the local pore structure and the stability of the water cluster –droplet network (see Figure 1).

Participation:

In-Person

References:

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MS04 / 529

A fully coupled hydro-mechanical modelling for describing gas transport in coal matrix

Authors: Ahmad MOSTAFA[None]; Luc Scholtes[1]; Fabrice GOLFIER[2]

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Coal bed methane (CBM), also known as coalbed gas, has drawn much attention lately as an alternative energy resource. Production curves of CBM reservoirs are very different, however, from the ones of hydrocarbon conventional reservoirs (Wang et al., 2011). As emphasized by several studies (Mostaghimi et al., 2017), transport and poromechanical properties of coal are strongly driven by topological and morphological features of its pore space.
The cleat-matrix system compartmentalizes the transport and mechanical properties of coal. Knudsen and surface diffusions prevail in the nanometer-sized pores of the matrix, while molecular diffusion and two-phase Darcy flow occurs mainly within the cleat network. All these transport mechanisms induce mechanical couplings related to both (i) the pore pressure changes which may alter the effective stress and consequently impact the bulk volume of the coal and (ii) the sorption processes which contribute to swell or shrink the coal matrix (Bertrand et al., 2017). The inherent couplings between the physical processes at stake and the multiscale features of coal need to be explored further to better assess the macroscopic response of the coal matrix and the sorption induced volumetric deformation.
We present a 3D model coupling a discrete element model and a pore network model specifically developed to describe the different diffusion mechanisms involved in coal matrix as well as the associated adsorption induced deformations. The material is assumed to be saturated with gas and diffusion occurs through the combination of Knudsen diffusion within the pore space, surface diffusion at the solid surface, and adsorption-desorption at the pore-solid interface. The model is hydro-mechanically coupled in the sense that changes in pore pressure produce hydrostatic forces that deform the solid skeleton, while deformation of the pore space induces pore pressure changes that promote interpore flow. Sorption induced deformations are taken into account by considering an additional pressure term related to the concentration of gas within the medium (the so-called solvation pressure). The implemented transport models are verified against analytical solutions describing diffusion in porous media with and without sorption-desorption, and a comparison is made with a swelling experiment performed on a coal specimen to illustrate the relevance of the proposed approach for describing adsorption induced deformation.

Participation:

In-Person

References:

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Poster / 530

Controlling colloid transport through porous media via local gradients of solute concentration

Authors: Mamta Jotkar[1]; Ilan Ben-Noah[2]; Juan J. Hidalgo[1]; Marco Dentz[3]; Luis Cueto-Felgueroso[4]

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Diffusiophoresis [1, 2] referring to the colloidal particle migration triggered by gradients of local salt concentration, has been established in the recent years as an efficient particle manipulation tool in relatively simple microfluidic setups such as plane channels [3], dead-end pores [4], Y-shaped channels [5], vertical diverging pores [6], etc. Owing to the fact that the particle velocities depend logarithmically on the solute concentration gradients, small variations in the concentration fields can result in significantly large diffusiophoretic particle motion [2]. However, despite the recent investigations hardly anything is known about its effects in the field of flow and transport in porous media. Spatial heterogeneities and complex fluid-phase distributions are quite ubiquitously found across spatial scales ranging from pore-scale to field-scale. These have a strong impact on the flow and transport of dissolved solutes through porous media giving rise to rich heterogeneous solute landscapes that provide local gradients of solute concentration, a prerequisite for diffusiophoretic motion. Following this motivation, we perform pore-scale simulations to understand the effects of diffusiophoresis at pore-scale in partially saturated media for varying degrees of fluid saturation and quantify their impact on the macroscopic particle transport. We envision that by exploiting the heterogeneous solute landscapes, particle motion can be controlled in an efficient manner. Depending on the sign of the diffusiophoretic mobility, determined by the size and surface charge of the colloidal particle, localized particle entrapment or removal can be achieved systematically. Our results that are pioneer in the field of diffusiophoretic transport through porous media, will pave the way to attaining controlled particle manipulation through porous media.

Participation:

In-Person

References:

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MS23 / 532

The role of Stern layer ions in ionic transport in porous media

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Understanding the role of Stern layer ions is crucial for assessing the ionic transport in nanochannels at high ionic strengths. Currently, MD simulations are one of the most promising tools to offer a realistic picture of the ionic behaviour close to charged surfaces where the Stern layer is located [1,2]. Experiments (like streaming potential and titration), on the other hand, are modelled using mean-field theories, like the Poisson-Boltzmann [3-6]. In this work, we show how the results of experimental investigations, interpreted using mean-field theories can be used to validate the results of MD simulations.
Specifically, a charged amorphous silica surface in contact with an electrolyte will be considered. The Stern layer is defined as the layer that starts at the surface of the silica and extends to a position where Poisson-Boltzmann starts to be valid. In the Stern layer, which has a thickness of a few Å, it is impossible to assume that ions are point-like, as this leads, especially at high ionic strengths, to unrealistic ionic densities. To account for a Stern layer, it is customary, in mean-field models, to model this region of space as a capacitor. The difference between the electric potential at the silica surface and the electric potential at the end of the Stern layer is then said to be equal to the surface charge density divided by the Stern layer capacitance (in F/m^2). The value of this capacitance can be estimated by modelling either by titration or by streaming potential measurements, for this capacitance is the only adjustable parameter in the model. We will show, in a first step, how the value of this Stern layer capacitance influences the ionic transport in streaming potential measurements and affects titration results. In a second step, we will compare the value found for the Stern layer capacitance with the results obtained from MD simulations. As the Stern layer capacitance is a function of both the Stern layer thickness and its permittivity, we will be able to discuss the value of the relative permittivity in the Stern layer.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS13 / 533

Spontaneous and electrocapillary imbibition dynamics in nanoporous media

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Imbibition is important physics in nanoporous media, related to many energy and technology areas, e.g., fuel cells, water desalinization, bio-sensor, hydrology, hydrocarbon recovery, CO2 geo-storage, underground hydrogen storage, etc. The classic theory to describe the spontaneous imbibition dynamics is the Lucas-Washburn (L-W) equation, while the classic theory to describe the electrocapillary imbibition is the Lippmann equation and the Young –Lippmann (Y-L) equation. However, whether these classic theories are still valid at nanoscale have not been rigorously examined yet.
Therefore herein, we experimentally investigate the dynamics of spontaneous and electrocapillary imbibition in nanoporous media. For spontaneous imbibition in hydrophilic nanoporous media in the absence of evaporation, spontaneous imbibition height is linear with square root of time and a larger pore size causes a faster imbibition, which are consistent with the L-W equation; in contrast, for spontaneous imbibition in hydrophilic nanoporous media in the presence of evaporation, this linear relationship is deviated from linearity at early stages and a modified L-W theoretical model is derived to incorporate the evaporation effect. For electrocapillary imbibition in hydrophobic nanoporous media, counterintuitive voltage polarity dependence and electro-dewetting phenomena are observed, indicating that the Lippmann and the Y-L theory are invalid to describe the fundamentals of electrocapillary imbibition at nanoscale. Hence, the underlying mechanisms responsible for these two novel physics are explained by electrical double layer charging, Faradaic reactions and others.
These insights will provide significant guidance on various applications relevant to energy transition, such as energy storage and conversion devices, water desalination, batteries and fuel cells.

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In-Person

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Poster / 534

Atomistic Insights into the Droplet Size Evolution during Self-Microemulsification

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[1] *University of Oslo*

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Microemulsions have been attracting great attention for their importance in various fields, including nanomaterial fabrication, food industry, drug delivery, and enhanced oil recovery. Atomistic insights into the self-microemulsifying process and the underlying mechanisms are crucial for the design and tuning of the size of microemulsion droplets toward applications. In this work, coarse-grained models were used to investigate the role that droplet sizes played in the preliminary self-microemulsifying process. Time evolution of liquid mixtures consisting of several hundreds of water/surfactant/oil droplets was resolved in largescale simulations. By monitoring the size variation of the microemulsion droplets in the self-microemulsifying process, the dynamics of diameter distribution of water/surfactant/oil droplets were studied. The underlying mass transport mechanisms responsible for droplet size evolution and stability were elucidated. Specifically, temperature effects on the droplet size were clarified. This work provides the knowledge of the self-microemulsification of water-in-oil microemulsions at the nanoscale. The results are expected to serve as guidelines for practical strategies for preparing a microemulsion system with desirable droplet sizes and properties.

Participation:

In-Person

References:

Fu, Y.; Xiao, S.; Liu, S.; Zhang, Z.; He, J., Atomistic Insights into the Droplet Size Evolution during Self-Microemulsification. Langmuir 2022, 38 (10), 3129-3138.

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Energy Transition Focused Abstracts:

MS03 / 536

Single-phase flow simulations in large-scale fractured porous media : solver challenges

Authors: Michel Kern[1]; Géraldine Pichot[1]; Martin Vohralik[2]; Daniel ZEGARRA VASQUEZ[3]

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In the subsurface, fractures are discontinuities in the medium in the form of narrow zones. Fractures are very numerous and present at all scales, with highly varying sizes and permeabilities. The permeability of the neighboring rock matrix is generally about two orders of magnitude lower than that of the fractures. This is why fractures are preferential channels for flow and, therefore, play a vital role in a large number of industrial and environmental applications.

One commonly used geometrical representation of fractured porous media is the discrete fracture matrix model (DFM) in which fractures are represented as manifolds of codimension 1. The model for single-phase flow in DFMs is described in 1, where Darcy's law in the fractures includes an additional source term that takes into account the coupling with the rock matrix.

Meshing the fracture network is carried out thanks to a specialized surface mesh generator called *MODFRAC* [2]. The surface mesh is then used as input for a volume mesh generator named *GHS3D* [3]. We developed *nef-flow-fpm*, a mixed hybrid finite element (MHFE) code for simulating steady-state incompressible single-phase flow in 3D DFMs. The MHFE method is conservative and leads to a square, sparse, symmetric, positive and definite linear system. Both direct [4, 5] and iterative [6, 7] solvers are integrated in *nef-flow-fpm*. Our code has been validated on a test case from the benchmarks in [8].

Because of the growing geometric complexity in large fracture networks, test cases recently proposed in the literature are mainly 2D, or 3D but with a limited number of fractures. In this talk, with the help of *nef-flow-fpm*, we analyze the computational costs from simulations with fracture networks of increasing complexity. The goal is to assess the performance of the linear solvers mentioned before and the challenges they face. We propose large-scale test cases, up to 87 329 fractures, generated with a genetic algorithm [9]. As expected, direct solvers suffer from large memory consumption, while iterative solvers may need a large number of iterations. Thus, we conclude that it is necessary to develop a dedicated, robust and efficient linear solver for even larger networks with more than one million fractures [10].

Participation:

In-Person

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Poster / 538

Multi-Scale Assessment of Surfactant-Assisted Spontaneous Imbibition

Author: Jamal Alaamri[1]

Co-authors: Viswasanthi Chandra [2]; Hussein Hoteit [3]

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Hydrocarbon-rich unconventional reservoirs are vital resources for the anticipated growth in energy demand. Spontaneous imbibition is a primary mechanism for improving shale fracturing and wettability alteration treatments in these ultralow-porosity and permeability reservoirs. Therefore, enhancing the efficiency of spontaneous imbibition is crucial to achieving higher recovery and delaying the decline in production rates. This study assesses the potential of surfactant-assisted spontaneous imbibition at multi-scale lengths, including Darcy- and pore-scales.

The proposed methodology consists of three main phases: Surfactants assessment, Darcy-scale, and pore-scale spontaneous imbibition. In this study, we selected three surfactants representing three different types of surfactants: cationic, anionic, and zwitterionic. Surface tension, interfacial tension, and contact angle are determined during the surfactant assessment. Then, we performed Amott Cell spontaneous imbibition experiments for all the surfactants in addition to the baseline on Berea sandstone rock. Finally, we assessed the performance of surfactant-assisted spontaneous imbibition at the pore-scale level using CT imaging. A micro-flow cell was used to perform the flooding while imaging with the CT scanner.

All surfactants reduced the interfacial tension and had variable contact angle results. However, the surfactants overall did not improve the spontaneous imbibition in Berea rock compared to the baseline. Cationic surfactants are comparable to the baseline results, as contact angle measurements showed that this surfactant slightly increased the rock's hydrophilicity. The other surfactants reduced the capillarity performance, leading to lower spontaneous imbibition. Segmented CT images

were used to estimate the plugs' initial oil and water saturations. Wetting and nonwetting phases were labeled and quantified by voxel counts. The change in oil saturation in the matrix was then calculated over time. The constructed production curves showed variations in the performance of the surfactants in enhancing oil recovery. A thorough discussion is provided to correlate the Darcy-scale spontaneous imbibition with the pore-scale results.
New insights into the fundamental mechanisms of spontaneous imbibition with various surfactant types were obtained. The provided study demonstrated that pore-scale analysis could improve the interpretation of production curves obtained by conventional Amott cell experiments. Multi-scale assessment helps understand how different surfactants enhance or hinder the process of spontaneous imbibition, leading to more optimized recovery.

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In-Person

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Poster / 539

Simulation Study on Heat Flow Coupled Heat Transfer in Porous Media

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Aiming at the changes of temperature field and velocity field caused by high temperature and high pressure fluid injected into reservoir porous medium during heavy oil thermal recovery process, based on Darcy's law, thecoupled equation of heat flow in porous media was established by the finite volume method. Based on the REV-scale porous media model, the effect of permeability and volume fraction of porous media and the injection pressure of hot fluid during thermal recovery on the heat flow coupling heat transfer process in porous media was studied. The results showed that the effect of increasing the permeability on the heat transfer of porous media was better than increasing the inlet pressure, increasing the solid volume fraction and increasing the thermal resistance, resulting in a decrease in heat transfer. Increasing the pressure of the injected hot fluid could increase the heat transfer rate.

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Energy Transition Focused Abstracts:

MS03 / **540**

Intermediate-scale experimental study and modeling of effects of caprock fracturing on brine contamination of shallow aquifers during storage of CO2 in deep saline geologic formations

Authors: Tissa Illangasekare[1]; Jakub Solovisky[None]; Holly Moser[2]; Ahamed Askar[3]; Fučík Radek Fučík[4]

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Brine leakage resulting from induced fractures during CO2 storage in deep geologic formation from pressure buildup during injection or existing faults in the far field risk contamination of the shallow aquifers used for drinking and other economic activities. Our past investigations studied the effects of uncertainties in the hydraulic parameters of the storage zone on the plume development and methods for optimal monitoring of leakage and pressure release through brine extraction. One of the main challenges in validating such methods is the unavailability of field data, as no such events have occurred. In our past and ongoing research, for these types of problems, we have used intermediate-scale testing systems where some field complexities can be mimicked to generate high spatially and temporally resolved data under highly controlled laboratory environments. This paper presents a study of the effects of uncertainties of the caprock fractures on brine plume development using this approach. A novel intermediate-scale testing system was developed to couple a fractured caprock to a geologic formation with two overlaying aquifer layers representing the shallow and intermediate zones over the caprock. The fracture network was designed using predefined geostatistical parameters, and a realization of the random network was etched into a plexiglass sheet. The etched channels were filled with sand to obtain the needed transmissivities to create a hydraulic leakage pathway. By injecting tracers at four different fracture initiating points, it was possible to activate different leakage pathways and plume configurations. The 1.3m x1.3m fracture zone was hydraulically connected to the eight-meter-long soil zone with the shallow and intermediate aquifer layers. The aquifer was packed with six well-characterized test sand types to create spatially correlated random fields for the two zones with different mean and variance of the log hydraulic conductivities. Bromide was introduced as a tracer representing the leaking brine, and the plume along the intermediate stratigraphic zone was tracked through aqueous sampling. Aqueous sampling in the shallow zone was performed using a high spatial resolution grid with 448 ports. The data collected for four leakage scenarios were used to validate and verify a new numerical model that couples the fracture and the aquifer zones to simulate the migration of the leakage plume. The model was used to conduct the uncertainty analysis by varying the parameters of the fracture zone represented as an equivalent porous medium. This paper presents the experimental system design, the coupled model, and the results from the uncertainty analysis.

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Energy Transition Focused Abstracts:

Poster / 541

Distributed sensing for monitoring greenhouse gas loading to the atmosphere through disturbed soil: Intermediate-scale testing

Authors: Tissa Illangasekare[1]; Ana Maria Ilie[1]; Yaobin Yang[2]; Kenichi Soga[2]; Richard Whalley[3]; Adriana Torres-Ballesteros[3]; Xiaoxian Zhang [3]; Trautz Andrew[4]

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The fundamental hydrologic processes that govern soil moisture dynamics in the vadose zone have a dominant effect on the transport and atmospheric loading of key greenhouse gases contributing to global climate change and related water issues worldwide. Drivers such as precipitation and heat and mass fluxes at the land surface impact vadose zone soil moisture distribution, which control the transport pathways and rates of water vapor and other greenhouse gases. A combined laboratory and field study is in progress to develop and apply a spatially distributed sensing technology to be used in agricultural and other plant environments. A part of this study is to test integrated sensing technology that uses embedded and fiber optics-based sensing and wireless sensor technologies under various soil and climatic conditions. Testing was done in an intermediate-scale three-dimensional porous media tank (4.2m x 2.4 m x0.42, where the temperature and water mass flux boundary conditions can be controlled. These tests will be upscaled to a longer test length of ~8 m in a coupled porous media and climate-controlled wind tunnel facility where the climate conditions in the near-surface boundary layer can be controlled. The goals of the tank experiments were to develop test methods and to test the hypotheses that fractures in soils will enhance greenhouse loading from the subsurface generated from geo-biochemical reactions. The tank was packed with a heterogeneous configuration using five well-characterized uniform silica sands with the effective sieve numbers #110, #70, #30, #40/50, #20/30, and #12/20, respectively. Spatial and temporal variations of soil moisture were monitored using embedded soil moisture sensors. A layer of silt with a high clay content was placed on the topsoil surface with the goal of creating thermal fractures using heat lamps. The silt layer was instrumented with fiber optical cables at two depths to monitor the fracture propagation from the soil surface into the silt layer. In two separate experiments, methane and CO2 were injected at the bottom of the tank using a distributed set of ports and allowed to migrate through the heterogeneous formation, and the gas concentrations at the soil surface were measured using three soil-gas flux chambers. The gas concentrations were also measured within the soil profile. In addition to the soil moisture sensors within the tank, the soil water tension within the silt was recorded continuously using precision micro tensiometers with the least disturbance to detect moisture variations during crack development from drying. The findings suggest that the testing methods were successful, and the data will allow testing the hypotheses on whether the fractures affect the gas loading to the atmosphere. The generated data will be used to validate numerical models to further testing of this hypothesis under possible field conditions and climate scenarios.

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References:

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MS15 / 542

Pseudo 3D unpaired domain transfer network for digital rock domain adaptation

Authors: Kunning Tang[1]; Ying Da Wang[1]; Peyman Mostaghimi[1]; Ryan Armstrong [1]

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Analyzing the physics under the same imaging condition is hampered by the domain difference between digital rock images from micro-computed tomography (micro-CT). Different scan devices, scan conditions, and sample conditions (dry/wet samples) are frequently to blame for domain differences in micro-CT rock images. Unpaired domain transfer by Generative Adversarial Network (GAN) is a method that reduces domain differences by transferring the image style from one to another without the requirement of paired images. Herein, we develop a pseudo-3D domain transfer network, Pseudo-3D Semantic CycleGAN (3D-PSCycleGAN) that transfers the rock domains with the user-defined semantic information in a 3D manner while only requiring 2D computational resources. The 3D stacking effect that is present in 2D networks without fail is eliminated by the pseudo-3D transmission. The 3D-PSCycleGAN opens up a way to analyze digital rock images under the same condition to avoid any bias or inconsistency.

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Poster / 543

Electrokinetic in situ recovery of copper: The influence of mineral occurrence, zeta potential, and electric potential

Authors: Kunning Tang[None]; Zhe Li[1]; Ying Da Wang[2]; James McClure[3]; Peyman Mostaghimi[None]; Ryan Armstrong[None]

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Hypothesis: in-situ recovery is an alternative to conventional mining, relying on the application of an electric potential to enhance the subsurface flow of ions. The governing physics of electrokinetic transport are electromigration and electroosmotic flow, which depend on the electric potential and excess charge adhered to mineral surfaces, respectively. Hence, mineral occurrence and its associated zeta potential should be the governing parameters that affect the efficacy of EK-ISR. Theory and Simulations: The governing model includes three coupled equations: (1) Poisson equation, (2) Nernst–Planck equation, and (3) Navier–Stokes equation. These equations were solved using the lattice Boltzmann method within X-ray computed microtomography images. The effects of mineral occurrence, zeta potential, and electric potential on a complex 3-dimensional synthetic iron ore were evaluated. Findings: Although the positive zeta potential of chalcopyrite can induce a flow counter to the direction of electromigration, the net effect is dependent on the occurrence of chalcopyrite. However, the ion flux induced by electromigration was the dominant transport mechanism, whereas electroosmosis made a lower contribution. Overall, Electrokinetic in-situ recovery is a promising technique that can be controlled because the dominant ion transport mechanisms are electromigration and diffusion. The former term depends on the applied external electric potential, and the latter term depends on the lixiviant injection.

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MS02 / 544

Combining floods and droughts - Mitigation of the effects of climate change on the local water balance

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Recent years have recorded an increase of the rainfall intensity which is met by a reduced infiltration capacity causing severe surface runoff, flooding, and groundwater depletion. Thus, the ecosystem functions of groundwater aquifers are at risk. The project Smart-SWS couples flood protection and drought management by infiltrating flood waves into porous aquifers close by (Flood-MAR). The water held back in flood retention basins is conditioned in the infiltration ditch to meet the quality criteria for groundwater recharge. Laboratory experiments to select suitable materials for the conditioning of the infiltrated waters are run. Here, the focus is on the removal of colloids and particles. As the infiltration is at irregular time intervals, we expect and test extended drying periods. A GIS-based site selection scheme has been developed and applied to select pilot sites. It respects (hydro)geological features as well as all kinds of protection zones and agricultural, municipal, and industrial use cases. To meet the pronounced asymmetry of infiltration (rapid infiltration requires high hydraulic conductivity) and long term storage (works best with low flow velocities) geotechnical measures like sheet pile walls or sand/cement injections are required. The concept is based on a minimum invasive approach: groundwater flow should not change at normal conditions and stagnation of groundwater has to be prevented. A hydrogeochemical model is developed to assess the reactions along the infiltration path and their effects on the integrity and stability of the aquifer.

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Poster / 545

Investigating calcite dissolution and relative effects on Underground Hydrogen Storage (UHS) through pore-scale reactive transport model and reservoir simulation

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Underground Hydrogen Storage (UHS), as an emerging large-scale energy storage technology with great compatibility with hydrogen economy, is at the centre of research attention in recent years. To investigate the feasibility of implementing UHS in porous reservoir such as aquifer or depleted hydrocarbon reservoirs, geochemical reactions brought by the presence of hydrogen in subsurface and their influence on hydrogen loss and reservoir integrity is heat-debated by many researchers. Among these geochemical reactions, calcite dissolution is one of the most important as it can not only affect the petrophysical properties of rocks, bring about substantial hydrogen loss, but also raise the pH value and release CO2 which trigger more biotic and abiotic reactions. There are already many experiment and modelling studies focusing on this topic. However, none of these studies succuss to model this reaction in a physical dynamic setting, leading knowledge gap between simulation results

and experiment observation. This is because the current models describing fluids-solid reactions are using ad-hoc surface area parameters during the reaction process. The influence from ion movement raised by surface charge and convection pressure gradient are also ignored. Herein, we use a novel pore-scale reactive transport solver by coupling fluid flow with geochemical reaction. The governing equations includes: (1) Poisson equation, (2) Nernst-Planck equation, and (3) Navier-Stokes equation. These equations were solved using the lattice Boltzmann method within X-ray computed microtomography images for a sandstone reservoir containing 10 vol% calcite, where Phreeqc is used to simulate geochemical reaction. By doing so, the effects from real-time pore morphology and mineral surface charge on the calcite dissolution kinetics, for the first time, are investigated under a transient condition. This study provides fundamental information on UHS in reservoirs containing sensitive minerals and facilitate the screening of potential UHS sites.

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Poster / 546

Enhancing Oil Recovery from Carbonate Reservoirs with Nanoparticle-Assisted Foams

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Due to its benefits of miscibility and diffusivity with oil, which results in recovering most of the oil within its swept zone, gas EOR is typically used to reduce decline in oil production. However, gravitational segregation, gas channeling, and viscous fingering are frequent occurrences during gas EOR operations. This results in a low mobility ratio and poor volumetric sweep efficiency, which adversely affect oil production, particularly in highly heterogeneous deposits. Foaming the injected gas, either by generating it in-situ or by alternating injection cycles of foaming solution with the gas, is a typical technique for preventing these issues. In order to reduce fingering, foams are generated to flow deeply within the formation layers. Furthermore, foams migrate into relatively small pores to block highly permeable layers and divert gas flow to establish a more uniform propagating front. This is key to improving volumetric sweep efficiency. With all these beneficial qualities of foam, it must remain stable in the porous media to produce positive results. Nanoparticles are positioned to be the focus of research related to foam stabilization, even under harsh reservoir conditions. In addition to increasing stability, surfactants and nanoparticles enhance foam EOR by the combination of their abilities to alter wettability, decrease IFT, decrease oil viscosity, and mitigate asphaltene deposition. In this work, a more specific and realistic foam investigation was carried as it was designed for an existing carbonate geological deposit, located in Volga-Ural region, Russia. In this work, a more specific and realistic foam investigation was carried as it was designed for an existing carbonate geological deposit, located in Volga-Ural region, Russia. An advanced technique of

high-pressure microscopy (HPM) was used to examine the stability of N2 and CO2 foams at reservoir conditions in the presence and absence of nanoparticles. The experiments were carried out at vapor and supercritical conditions. Furthermore, core flooding studies were performed to investigate their effect on oil displacement and mobility control in both real and artificial core samples. Our results indicated that foams produced at 80% quality were more stable than foams produced at 50% quality because the bubble size was significantly smaller while bubble count was higher. Additionally, foams under supercritical conditions (sc) exhibited greater stability than foams under vapor conditions. This is because at supercritical conditions, gases have a density similar to that of liquids and this helps to strengthen the foam lamella by enhancing the intermolecular contacts between the gas and the hydrophobic part of the liquid phase. In the core flooding experiments, an initial displacement efficiency of 48.9% was recorded for scCO2 and the use of foam allowed us to increase the total displacement efficiency up to 89.7% in the artificial core model. In the real core model, CO2 foam injection increased oil recovery during CO2 injection from 37.7% to 66.6%. The results of this study showed that nanoparticles-enhanced foams have the beneficial potential for EOR purposes and for the mitigation of early gas breakthrough which was noticed after injecting about 0.14 PV during scCO2 injection.

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Energy Transition Focused Abstracts:

MS01 / **547**

Sensitivity Analysis of CO2 Mineralization Trapping during CO2 Sequestration

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One of the toxic greenhouse gases that significantly alters the climate is CO2, and it may be possible to lower its emission by sequestering it in an appropriate geological subsurface formation. For a secure and effective sequestration, it is necessary to answer questions relating to enhancing the reaction rates of rock minerals to speed up sequestration, understanding the critical reservoir parameters involved with geochemically induced changes and how they affect mineralization, and the affinity of rock minerals for dissolution or precipitation in the presence of CO2 and reservoir brine. Depleted oil and gas fields and deep saline aquifers are the most practical storage locations, while the latter is preferable because it is widespread and has a great storage capacity. However, inadequate rock mineral assessments, heterogeneities in the underlying characteristics, and insufficient knowledge of CO2 geochemical reactivity with in-situ minerals are some of the major obstacles to its development for CO2 storage. Hence, this study focuses on mineralization trapping mechanism of CO2 by simulating the sequestration of at least 48 million tons of CO2 over a five-year period

in a saline aquifer. The effectiveness of CO2 mineralization trapping for the siliciclastic aquifer formation was characterized in relation to the impacts of injection period, pressure, temperature, and salinity. The ability of the aquifer to inject, mineralize, and store significant amounts of injected CO2 for a duration of 1000 years was studied using a numerical simulator. This study also analyzed the geochemical induced changes such as pH and porosity changes that occurred due to mineralization. Our results showed that while increasing the injection period appears to increase the efficiency of CO2 mineralization trapping, this is only the because there is more CO2 available in the formation, as a comparison with the volume of CO2 injected yields a contrary result. Additionally, the findings in this work can provide the appropriate mineralization temperatures at which each of the simulated minerals can either dissolve or precipitate. Calcite and dolomite mineralize more effectively at medium and lower temperatures, despite the fact that reaction of other minerals such as illite, kaolinite, k-feldspar and quartz will be more favored at high temperatures. Porosity and pH showed only slight variations, but they were sufficient to indicate the dynamics of mineral reactivity and mineralization trapping efficiency.

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549

Fingering Instabilities in a Radial Hele-Shaw Cell with Wettability Heterogeneities

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Fingering instabilities develop when a low-viscous fluid displaces a high-viscous fluid in porous media. Fingering promotes deep contamination of groundwater, limits the efficiency of hydrocarbon recovery and geological CO2 storage, and creates non-uniform coatings. Classical Hele-Shaw studies on viscous fingering have not addressed the role of surface wettability heterogeneity, a common property of many natural and engineered solid surfaces. Wettability defects affect features of wetting dynamics, including contact line pinning and residual wetting films. These features may influence the flow behavior and fingering instabilities in Hele-Shaw cells.

This study aims to investigate the effect of wettability heterogeneities on flow behavior in Hele-Shaw cells, with specific attention to fingering phenomena. We construct radial Hele-Shaw cells with patterned solid surfaces containing wettability heterogeneities. The wettability defect is treated using a

commercial silane water repellent and has a water/air contact angle = 97compared to a = 29 for a clean glass surface. We use a stencil cutting machine to create stencil patterns, which enables effective wettability patterning of a large surface area. Then we conduct fluid displacement experiments in the cell and analyze the fluid flow control mechanisms exerted by wettability heterogeneities. A syringe pump (Chemyx Fusion 200) maintains a constant injection rate, and a digital camera (Nikon, D5500) positioned over the radial Hele-Shaw cell records the displacement. Experiments consider the effects of the density and distribution of wettability heterogeneities, flow rates, and fluid pairs (air and water/glycerol, water and mineral oil) on fingering phenomena.

Results show that uniformly/randomly distributed wettability defects can roughen the advancing front, broaden finger growth regions, and increase displacement efficiency for the condition of air injection into a water/glycerol mixture. However, the distribution and orientation of wettability heterogeneities also determine whether viscous fingering will be suppressed or promoted. Fingers are promoted and narrower in cases where elliptic wettability defects are oriented radially, and the displacement efficiency Ef can be as low as 0.508. However, defects perpendicular to the flow direction suppress finger growth and can increase the displacement efficiency to as high as Ef = 0.936. A lower flow rate supplements the effect of capillarity and wettability, thus strengthening the impact of wettability heterogeneities. More surprisingly, stable displacement instead of viscous fingering is observed when water injects into a more viscous mineral oil in Hele-Shaw cells with wettability heterogeneities. We present a linear stability analysis that attempts to explain this phenomenon.

Our experiments provide insights into the wettability control on fingering behavior in porous media and have implications for a number of industrial applications, such as the interpretation of core flooding data, reservoir applications involved during geological CO2 storage and hydrocarbon recovery, as well as potential manipulation of fingering phenomena in microfluidics and advanced porous materials.

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MS09 / 550

Wettability effect on flow-driven deformation using hydro-mechanically coupled pore network model

Author: Min-Kyung Jeon[1]

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Wettability has an enormous impact on the effectiveness of enhanced oil recovery (EOR) techniques and geologic carbon storage (GCS). Water flooding or carbon dioxide injection in EOR or GCS imposes pore pressure on the media, which can induce deformation or even failure of porous media. Experimental studies have shown that wettability is a key factor in determining flow patterns along with fluid characteristics and injection conditions. However, most previous research has been conducted in non-deformable media. As some studies performed in deformable media are limited to macroscopic scale, pore-scale study on simultaneous deformation or failure by immiscible flow is still lacking. This study attempted to examine the effect of wettability on hydromechanical behavior using pore-scale modeling. Fluid injection pressure alters the porous structure by mechanical deformation, causing a change in flow characteristics with the re-distribution of pore pressure. Therefore, a two-way coupling between hydraulic and mechanical behavior is required to mimic this process. To achieve two-way coupling, force equilibrium at each node was assumed in pore network model and block-spring model. Flow pattern and mechanical behavior under various wettability were explored using a two-way hydro-mechanically coupled pore network model.

Acknowledgment
This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant, funded by the Korean Ministry of Trade, Industry & Energy (No. 20212010200020)

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Poster / 551

Fracture matrix pore network model (FM-PNM): an efficient pore scale modelling method of fluid flow in fractured porous media

Authors: Chenhui Wang[1]; Kejian Wu[2]; Gilbert Scott[3]; Ailin Jia[1]; Yunsheng Wei[1]; Zhi Guo[1]

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Fluid flow in fractured porous media is concerned with various processes in science and engineering, including transport, chemical and mechanical processes, etc. Direct numerical simulations of fluid

flow can investigate pore-scale processes and flow mechanisms in fractured permeable media. However, the tremendous computational costs prevent these methods from being applied to larger-scale models. On the contrary, pore network modelling is efficient and applicable to simulate large-scale porous media and handle thousands or even millions of pores simultaneously (Blunt, 2017). But currently, the pore network method can only be used in porous media without fractures.

In this work, we propose a new model to explicitly incorporate fractures into pore networks to represent fractured porous media. A new fracture matrix pore network model (FM-PNM) is developed to efficiently simulate the fluid flow properties in fractures associated with the pore matrix. The fractures are simplified as ideal planar cuboids with properties of aperture, width, length and orientation, which are then transformed into fracture pipe networks. The pore matrix is represented by a topological network of pore bodies (nodes) connected by pore throats (bonds). These two networks are coupled together to create a single nested network which is topologically equivalent to the fractured porous medium. The permeability of the coupled network (FM-PNM) is benchmarked by Lattice Boltzmann simulation for various structures of pore matrix and discrete fracture networks (Latt et al., 2020). A reasonable agreement was achieved which demonstrates the value and efficiency of the fracture matrix pore network model.

Participation:

In-Person

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MS17 / 552

Model Development for Thermal Management of Li-Ion Batteries from Cell Level to Total System Level

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Li-Ion batteries are widely used for energy storage mediums because of their high volumetric and gravimetric energy capacities and proven mature technology level suitable for mass production. However, they have one key problem which is the heat generation during charging and discharging cycles. As the cells are getting too hot or too cold, battery life and performance decreases. If the heat generated from the batteries are not dissipated, there is even risk of explosion. To model the thermal behavior of the battery package one first needs to figure out the heat dissipated from a single cell, which can be set as an heat source value for the thermal modeling for the battery package. This can

also be achieved with electrode scale continuum scale models, where Li transport in electrolyte and charge balance and Li diffusion in porous electrodes are modeled. However, electrode scale model would be over detailed to combine with a system level model.
First, cell level 2nd degree Thevenin's equivalent circuit model 1 was developed under Matlab (fig. 1 and fig.2).

Figure1. Thevenin's equivalent circuit model concept

Figure2. Thevenin's equivalent circuit model developed under Matlab

The model requires Open Circuit Voltage (Uoc) vs State of Charge (SOC) relationship as an input. The parameters Ro represents contact/ohmic resistance of the cell, R1-C1 represents cell polarization, R2-C2 represents diffusion process [2], which are determined by fitting terminal voltage (Ut)-SOC measurement. Different from the lead acid batteries the Li-Ion cells have exponential decrease in the terminal voltage when the terminal voltage is approaching the cut-off voltage. To mimic this behavior, the equivalent circuit components (R,C values) are not set to constant values, they are varying as a function of SOC.
The developed Thevenin Model is able to calculate SOC, Uoc, Ut, state of health (SOH), remaining capacity, useful capacity [3], thermal power and generated heat. The main purpose of building an equivalent circuit model is to calculate thermal power generated by the cell (Thermal_Power=(Uoc-Ut)* I_current) [4,5].
Battery Package level simulation is carried out with setting thermal power of Thevenin model as a heat source to model temperature distribution. Thermal conductivity properties are taken from [6]. This is achieved with Comsol finite element simulation software (fig. 3).

Figure 3. Temperature distribution within the battery package with active air cooling

Total system model is created to model system dynamics with varying terminal current. Total system model is composed of Grid Connection, Auxiliary Load, Power Control System, Power Management System, Convertors, HVAC System, Battery Management System and Battery Package. The developed equivalent circuit cell module is set in the heart of the battery package module. During operation the main heat sources are battery packages. The temperature distribution of the total system is calculated with FEM simulator.

The advantage of this approach is that the experimental data can be perfectly fitted to the model data. The drawback of this approach is that the heat that is generated during charge/discharge process is assumed to be homogenously distributed at the outer surface of the cell.

Participation:

In-Person

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MS06-B / 554

Adsorption, ion exchange, and surface complexation models for rock-fluid-fluid interactions: an overview and a new implementation in REAKTORO

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The adsorption of ionic species at the interfaces between rock and brine, and between brine and non-aqueous phase liquids (NAPL) such as crude oil, can significantly impact the mobility of these substances in porous media. In this work, we present a set of simple benchmarks to evaluate the accuracy and consistency of existing mathematical models and thermodynamic software in predicting the chemical interactions at these interfaces. We also propose a new open-source implementation of surface complexation models in REAKTORO with practical applications in enhanced oil recovery (EOR), carbon capture and storage (CCS), and ground water remediation. These models, which take the form of Langmuir isotherms in their simplified form, are commonly used to model rock-brine interactions and explain experimental observations such as electrophoretic mobility, streaming potential, and chromatographic retention of ions. However, there is currently no systematic comparison among the various forms of surface complexation models and their numerical implementations. To address this gap, we suggest a range of rock-brine mixtures including natural and artificial calcite, sandstone, and clay minerals in contact with brines of different compositions, and solve these systems using Langmuir, ion exchange, Constant Capacitance (CC), Diffuse Double Layer (DDL), Triple Layer (TL), and Charge-Distribution Multisite Complextion (CD-MUSIC) models in Phreeqc, Geochemists Workbench, Visual Minteq, and ORCHESTRA. We compare the results with our own numerical and analytical solutions. In addition, we present a general formulation of surface complexation models in REAKTORO, addressing issues with the existing numerical implementations related to the explicit calculation of the double-layer composition and the assumptions made about the thickness of the double layer. Our new implementation and benchmarks provide a comprehensive, consistent, and numerically efficient framework for modeling interactions between charged interfaces and their impact on multiphase flow and mechanical behavior in subsurface porous media.

Participation:

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Poster / 555

An experimentally validated conceptual model for numerical simulation of accelerated dissolution trapping of CO2 in low-permeable fractured reservoirs

Authors: Ali Akbar Eftekhari[1]; Yao Xu[2]; Yibo Yang[1]; Wei Yan[1]

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The dissolution trapping of CO2 in water, often accelerated by gravity-driven convection of overlying CO2 plume in high permeable water-saturated rocks, can ensure safe long-term sequestration of CO2 but can take thousands of years in low permeable rocks (< 1 mD). We hypothesize that in naturally fractured reservoirs, even with low to no fracture network connectivity, the density-driven convective flux of CO2 in the water-saturated vertical fractures can reduce the required time for dissolution trapping to several years to few decades depending on fracture density. We validate the numerical model with pressure decline curves obtained in a novel experimental setup, in which the lateral area of a brine-saturated low-permeable chalk core (< 1 mD) is in contact with supercritical CO2 in a closed PVT cell at reservoir temperature and pressure of a Danish North Sea chalk field. Our model consists of CO2 transport with advection and diffusion and the continuity equation for a slightly compressible system of brine with dissolved CO2. The solubility of CO2 and the density of CO2-water mixture are modelled with Phreeqc, which utilizes the Peng-Robinson equation of state for the fugacity of CO2 and water in the gas phase and the Pitzer model for the activity of CO2 and other ions in the aqueous phase. We also use the default values of partial molar volumes in the Phreeqc database and validate the results against published experimental data for CO2-brine solubility and density. We then solve the equations both in our in-house finite volume solver (with TVD scheme for the advection term and backward Euler for time) and COMSOL multiphysics (finite element with added artificial diffusion for numerical stability). We model the 2D dissolution of CO2 in a water saturated fracture (with rough surfaces) and show that for a fracture aperture in the range of 0.03 to 3 mm, a long fracture will be filled with CO2-saturated brine in less than a few days. We then show that these saturated fractures serve as boundary conditions for fast dissolution of CO2 in the low-permeable matrix with diffusion-controlled mechanisms for permeabilities less than 1 mD and convection-dominated flow for permeabilities higher than 10 mD. We also discuss the implications of the results on the capacity of the Danish waterflooded chalk reservoirs for the storage of CO2 without displacing the formation fluids, which is currently not allowed in Denmark.

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MS09 / **556**

Representation of Fully Three-Dimensional Interfacial Curvature in Pore-Network Models

Author: Luke Giudici[1]

Co-authors: Ali Qaseminejad Raeini [2]; Martin Blunt [3]; Branko Bijeljic [1]

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Quasi two-dimensional approximations of interfacial curvature, present in current network models of multi-phase flow in porous media, are extended to three dimensions. The effect of each principal radii of curvature on displacement is analysed using high resolution direct numerical simulations on synthetic geometries, for both uniform and mixed-wet wetting states, and the analysis is used to calibrate network model extensions. A fully three-dimensional consideration of interfacial curvature is shown to be a key step in improving the physical accuracy of network models. Finally, the calibrated network model is used to obtain predictions of relative permeability and capillary pressure for a water-wet and a mixed-wet Bentheimer sandstone, and compared to experimental measurements, where the inclusion of three-dimensional interfacial curvature yields more accurate predictions.

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MS04 / **557**

Influence of interaction between confined hydrogel beads on their growth swelling dynamics

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Hydrogels are polymeric materials that can absorb large amounts of water, swelling and increasing considerably in size. They are used in a wide range of applications, including some in which the hydrogel is required to absorb liquid under pressure. For example, for soil remediation and water storage in agriculture, hydrogels maybe located deep underground and must withstand the mechanical stress from the soil while swelling the water and at the same time absorbing any heavy metal ions present in the soil.
In this work we study the influence of confinement and interaction between hydrogels beads during their swelling. A large cylindrical vessel was used, where a single hydrogel can swell freely without interaction with the side walls. A initially dry hydrogel bead, diameter (2.8 ± 0.2) mm, is submerged in an aqueous solution containing a small amount of dissolved fluorescein, which allows UV light visualization but does not affect the swelling. A top piston is placed in contact with the hydrogel. The piston can move vertically with negligible friction until it reaches a force sensor at a fixed and controllable height H. H determines the vertical confinement and is varied between 4 and 12 mm. The force exerted by the hydrogel on the piston is measured during swelling. Three different kinetic regimes were identified in the swelling of a single hydrogel bead, independent of the confinement H: 1) "flower like" swelling, in which the hydrogel bead presents a dry core surrounded by a wet shell of wavy geometry due to a surface instability; 2) isotropic and homogeneous swelling and 3) confined swelling, after the hydrogel bead reaches a size equal to H and swells under compression in the vertical direction. The force exerted by the hydrogel bead on the piston was found to increase with confinement (as H decreases). The pressure exerted by the hydrogel bead on the piston agrees with Maxwell's viscoelastic model at constant strain. The measured pressure and deformation at long times show an elastic behavior for all the values of H studied. Finally, the influence of interactions between hydrogels in confined media is studied varying the total number of hydrogels beads (NH) between 5 and 30. It is observed that, for a given H, the force exerted on the piston increases with the number of hydrogel beads present in the cell. However, the total force depends linearly on the number of hydrogel beads until NH=20.

Participation:

In-Person

References:

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MS03 / 561

About long time asymptotic solutions of non-linear counter current two-phase flow in rock matrix blocks

Authors: Benoit Noetinger[1]; Frédéric Douarche[1]; Benjamin Braconnier[1]; Sina Momeni[1]

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Counter-current flow can be encountered under quite general conditions in two D or 3D two-phase flows in fractured medium. It may describe the imbibition of a wetting fluid replacing a non-wetting fluid inside the rock matrix. As the first order term of the driving transport equation drops-out, the resulting transport equation is a singular non-linear diffusion equation.
Although the early time solution of such equations is quite well known, it turns out that the long-time asympotics describing the asymptotic decay of the overall non-wetting fluid saturation is less known.
In that contribution, we develop a general self-similar solution, the time dependance of which is a power law of time, with an expoennt related to the NAPL rel perm decay at law NAPL saturation. The spatial part of the solution can be computed using a suitable fixed point algorithm that solves a non-linear eigenvalue problem. In stratified media, a complete analytical solution can be developped. In the genral case, numerical tests performed with accurate complete simulations confirm the relevance of that solution for many matrix block shapes. Consequences about the matrix to fracture overall fluw are also expected.
As the convergence of the solution to its asymptotic appears to be quite slow, a perturbative approach was developped to get a firther understanding of that observation. That allows us to develop an asymptotic solution under the form of a series of time power-laws that may describe the NAPL overall saturation decay once lower than 40% of its initial value.
Such solutions may be used to look for physically based proxys of matrix to fracture exchanges well-suited for developping an averaged description when considering a population of matrix blocks of random sizes and shapes.
In that talk, we will present previous findings published in following paper, as well as more recent results. Douarche, F., Braconnier, B., Momeni, S., Quintard, M., & Nœtinger, B. (2022). Counter-current imbibition and non-linear diffusion in fractured porous media: Analysis of early-and late-time regimes and application to inter-porosity flux. Advances in Water Resources, 169, 104319.

Participation:

In-Person

References:

Douarche, F., Braconnier, B., Momeni, S., Quintard, M., & Nœtinger, B. (2022). Counter-current imbibition and non-linear diffusion in fractured porous media: Analysis of early-and late-time regimes and application to inter-porosity flux. Advances in Water Resources, 169, 104319.

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Poster / 562

Viscous coupling effect on hydraulic conductance in dynamic pore network model

Author: Wenbo Gong[None]

Co-authors: Yang Liu ; Ju Yang [1]; Wang Moran [2]

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Viscous coupling during simultaneous flow of different fluid phases has a significant impact on their flow through porous media. In this work, a new multiscale strategy is proposed for multiphase flow in porous media. We use the interfacial continuum equation to simulate two-phase flow at pore scale and obtain empirical terms for the viscous coupling inside individual pores under variaous wettability conditions, interfacial distributions, and viscousty ratios. The hydraulic conductance of different fluid phases is validated by comparison with the mobilities computed using the lattice Boltzmann modeling. The mean value of relative error in hydraulic conductance predicted from our empirical model is less than 1%, compared to the other viscous coupling equations with errors more than 11%. The empirical coupling terms are then used in a dynamic pore-network model to efficiently simulate two-phase flow through porous media at core scale. It is shown that including viscous coupling leads to better predictions of relative permeability.

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In-Person

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Energy Transition Focused Abstracts:

Poster / 563

Towards the prediction of caprock porosity and permeability for CO2 storage seal integrity assessment

Author: Wan Muhammad Luqman Sazali[None]

Co-authors: Andreas Busch [1]; Jingsheng Ma [1]; Jim Buckman [1]

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Carbon capture and storage (CCS) requires sealing caprocks to ensure the stored CO2 is contained in the reservoir and not leaking towards the surface. Many caprocks are composed of mudrocks, a siliciclastic sedimentary rock with a high clay content. We here analyse such a caprock from the Field S which is a potential CO2 storage site in the Sarawak Basin, East Malaysia. The determination of important caprock properties, like porosity and permeability, is often difficult and requires fresh core material that is adequately stored for lab testing. When such core material is not available, drill cuttings might be used as alternatives to predict formation properties if suitable empirical relationships are available which is the objective of this study.

Therefore, we performed a petrophysical characterisation of core and cutting samples using mercury intrusion porosimetry (MIP), unsteady state pulse decay permeameter, nuclear magnetic resonance and helium pycnometry measurements. Because of shape limitations, only MIP and helium pycnometry are suitable to determine porosity and permeability on drill cuttings, while plug samples can be used for permeability tests under subsurface stress conditions. In addition, we performed a full characterisation of the sample to obtain mineralogy, pore size distribution and grain sizes. Finally, the lab data has been correlated with well log data to further understand the porosity and permeability trend for prediction purposes.

Sedimentologically, we find that the caprock in Field S is divided into two facies (Seal A and Seal B) with varying clay contents of ~20 and ~40% respectively. In term of grain size distribution, this field is mostly dominated by fine silt (2.0 to 6.3 microns), with a higher fine silt content in the deeper Seal B. However, laboratory determined porosity and permeability do not vary significantly between these two facies, even though seal B has higher clay contents. This might be because Seal B is significantly over-pressured compared to Seal A, potentially resulting in porosity preservation during compaction and therefore increased permeability. This is consistent with the time-to-depth conversion from seismic data, where Seal B is identified as being undercompacted in comparison to Seal A. Porosity from MIP is generally lower than porosity from helium pycnometry, for both core samples and drill cuttings. This is because mercury invasion is restricted to pores >3 nm and therefore underestimates the total porosity. Additionally, porosity and permeability values determined on unconfined drill cuttings are always higher than the values measured on confined plug samples.

Here, we will present our workflow in predicting porosity and permeability of caprocks based on a petrophysical and mineralogical database developed for Seal A and B. We will discuss issues with this approach and its potential and highlight the difficulties in determining permeability from confined plug or unconfined cutting samples.

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In-Person

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Energy Transition Focused Abstracts:

Poster / 564

Applying Thermodynamic Framework to Analyze Transport Self-Organization Due to Dissolution/Precipitation Reaction in Porous Medium at Varying Peclet Number: Entropy, Enthalpy, Heterogeneity

Author: Evgeny Shavelzon[1]

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Dissolution/precipitation processes in reactive transport in porous media are ubiquitous in a multitude of contexts within the field of Earth sciences, such as geological hydrogen and carbon storage, reactive contaminant transport and acid injection in petroleum reservoirs. In particular, the dynamic feedback between the reactive process and solute transport, capable of giving rise to the phenomenon of preferential flow paths, is critical to a variety of Earth science scenarios, as these paths are responsible for the alteration of transport properties of the porous medium; still, the approaches to its characterization remain disputed. It has been argued that the emergence of preferential flow paths in porous media can be considered a manifestation of transport self-organization, as they introduce spatial gradients that distance the system from the state of perfect mixing.

To investigate the dynamic feedback between the reactive and transport processes and its influence on transport self-organization, we consider a 2D Darcy-scale reactive transport setup, where dissolution and precipitation of the porous medium are driven by the injection of an acid compound, establishing local equilibrium with the resident fluid and the porous medium, composed of a calcite mineral. The coupled reactive process is simulated in a series of computational analyses employing the Lagrangian particle tracking approach, capable of capturing the subtleties of the multiscale heterogeneity phenomena. We employ the thermodynamic framework to investigate the emergence of the preferential flow paths as the manifestation of transport self-organization; in particular, we are interested in the relationship between the Shannon entropy, used to quantify self-organization and the enthalpy.

We find that, for an initially homogeneous medium, transport self-organization increases with the evolution of the reactive process, along with the emergence of heterogeneity in the medium due to feedback between the reaction and transport. We identify the reciprocal of the Peclet number as the driving force for transport self-organization, as the stochastic nature of diffusion leads to inhomogeneity of reaction, resulting in the emergence of heterogeneity in the medium; this causes re-distribution of the transport, thus increasing its self-organization, as signified by a decrease in Shannon entropy. The decreasing entropy is accompanied by an increase in enthalpy due to an enhanced global reaction rate. The self-organization of the breakthrough curve exhibits the opposite tendencies, explained from the thermodynamic perspective. The energy, required to maintain self-organization within the thermodynamic framework, is supplied by the hydraulic power under the applied hydraulic head drop boundary condition; this power increases with the heterogeneity.

To conclude, our findings suggest that Peclet number of the transport has a crucial impact on the interaction between the reactive and transport processes in porous medium, as expressed in terms of transport self-organization within the thermodynamic framework; this has important implications for both hydrogen and carbon geological storage due to reactive processes that take place in the storage medium, caused by the altered pH level.

Participation:

In-Person

References:

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MS17 / 565

Heat Extraction at High Flow Rates by Fracture Plugging in Geothermal Reservoirs from Pore to Darcy Scale Considering Local Thermal Non-Equilibrium (LTNE) Conditions

Authors: Yashar Tavakkoli Osgouei[1]; Mehmet Onur Doğan[1]; Serhat Akin[1]

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The existence of fracture network in porous media can have positive or negative effects on matrix-fracture transfer depending on the flow rate. In higher flow rates the efficiency of heat extraction decreases in fractured geothermal reservoirs due to preferential flow through the fractures. The fracture plugging can be considered as a solution to cope with it by diverting flow through porous matrix, resulting in more heat extraction. In present study, the effect of fracture plugging on heat extraction was investigated by cold water injection through the single fractured core plug including an obstacle at different flow rates. Present study indicated that the presence of obstacle in the fracture contributes high heat extraction compared to the absence of it because of fluid penetration into matrix from fracture. The analysis of heat transfer in porous matrix by Local Thermal Equilibrium (LTE) conditions leads to overestimated outlet temperature, thermal analysis with Local Thermal Non-Equilibrium (LTNE) conditions is more accurate, especially, at higher flow rates. In LTE condition both solid and fluid phases are at the same temperature and the average porous media temperature can be scaled with porosity and heat capacities of the fluid and solid phases1. In LTNE condition fluid and solid phases have different temperatures. Energy balance equations of the phases are coupled with heat source terms described with interstitial heat transfer coefficient [2]. Numerical studies indicated that in Darcy scale the main controlling parameter is interstitial heat transfer coefficient between solid and fluid phases. Minkowycz et. al [3] investigated the effect of rapid heat source change on NLTE conditions via analytical solutions in Darcy scale. Wang et. al [4] studied NLTE conditions in porous media with trapped fluid - solid matrix system. At LTNE conditions, interstitial heat transfer coefficient of Darcy scale problem can be calculated by averaging heat flows over the solid - fluid interface in pore scale.
In the present study the single fracture-matrix system was selected for cold water injection mimicking geothermal system. Since we are focusing on geothermal energy, there is a flow in our present study, where the Darcy scale parameters are extracted from pore scale model. There is constant injection rate at the inlet and constant pressure at the outlet of the fracture. Other boundaries are no-flow boundaries. Coating the system with epoxy resin allows no flow conditions at the outer surface. Temperature at the outer surface is kept constant.

Fig. 1. Matrix- fracture model domain for thermal transport problem

At the same flow rate temperature of the solid matrix is lower in LTE compared to LTNE condition, which clearly shows an overestimate for heat extraction (Fig. 2). Whereas at the fracture outlet, temperature of LTE is larger, since in LTNE condition there is still a transient heat transfer between the solid and fluid phases. As the flow rate increases, temperature at fracture outlet decreases in both LTE and LTNE conditions (Fig. 3).

Fig. 2. Matrix temperature values for a) LTE and b)LTNE conditions

Fig 3. Fracture temperature output for LTE and LTNE conditions

Participation:

In-Person

References:

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Poster / 567

Mechanistic studies on the adsorption of Iodinated Contrast Media agents on Activated Carbon

Authors: Ashfeen Ubaid Khan[1]; Alberto Guadagnini[2]; Monica Riva[2]; Giovanni Porta[2]

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We focus on the evaluation of the adsorption energy (EAd) of 24 Iodinated contrast media agents (ICMs) on activated carbon through Density Functional Theory (DFT) in silico simulations. The study is motivated by the emergence of concerns related to the impact of pharmaceuticals on the environment and human health [1,2]. Iodinated contrast media agents are typically used in radiology, primarily in CT scans for soft tissue imaging [3]. Their presence in the environment can be the source of hazard [4]. With an annual global consumption of 3.5 × 106 kg [5], ICMs have been frequently detected in surface water bodies as well as in groundwater systems with levels up to 100 µg/L [3]. While conventional water treatment technologies are unable to contain the release of ICMs into the environment, some studies document the possibility that toxic by-products resulting from the transformations of ICMs can affect water and soil systems [3,6]. Thus, there is a growing need for robust technologies for the removal of ICMs from aquatic environments. Most of the available studies focus only on a few selected ICMs such as diatrizoic acid, iopamidol, or iohexol [3]. Considering that there are more than 30 ICMs available commercially [7], our study is the first one providing a comprehensive analysis of a variety of these compounds. Due to its tunable physiochemical properties, activated carbon is a porous material of remarkable interest in the context of groundwater remediation practice [8]. Because of the complexity and uncertainty associated with the structure of activated carbon, we use monolayer graphene as a proxy model [9,10]. We find that overall strong adsorption energies (EAd) can be documented through our DFT studies. These

range from -114 Kcal/mol for Iophendylate to -13 Kcal/mol for Methiodal. To enhance our knowledge about the fundamental mechanisms underpinning the adsorption of ICMs on activated carbon, we rely on a Quantitative structure-activity relationship (QSAR) regression modeling approach. The latter yields quantitative correlation between (a) chemical structure information which is, in turn, represented in terms of molecular descriptors, and (b) adsorption [11]. Our results suggest that descriptors such as the topological charge index and the Van Der Waals surface area (of aromatic atoms) are positively corelated to adsorption energy. Otherwise, other descriptors, such as, e.g., the 'average Randic-like index from Burden matrix weighted by ionization potential', are characterized by a negative correlation to EAd. Our results are intended as a first step to assist the assessment of the role of intermolecular interactions governing adsorption of ICMs on activated carbon surfaces and to enhance our ability to further improve (and possibly design) a new generation of porous media to be effectively employed as sorbents in this context.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 569

A color-gradient lattice Boltzmann model for fluid flow with high density and viscosity ratios

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Multiphase fluid flows frequently occur in nature and industrial applications including microfluidic devices, enhanced oil recovery, CO2 storage, etc. In order to have a better understanding of multiphase physics, several numerical methods have been developed over the past. The lattice Boltzmann method (LBM) as an alternative to the classical computation fluid dynamic (CFD) method has received much attention due to its favorable features over the classical CFD such as ease of implementation, highly scalable parallelization, and straightforward handling of complex boundaries. In the LBM framework, different models usually fall into four categories; the color-gradient (CG) model, the Shan and Chen (SC) model, the free energy model, and the mean-field model. Among these models, the CG model performs better in conserving mass and since its emergence, it has been advanced to tackle different multiphase physics.

In this paper, a new formulation of the color-gradient method is developed, and a solver based on the lattice Boltzmann (LB) framework is proposed to solve the new formulation. The macroscopic equivalent of the formulation is presented which makes the physical interpretation of the color-gradient easier. In contrast to existing color gradient models where the interface capturing equations are coupled with the hydrodynamic ones and include the surface tension forces, an available LB equation which is capable of handling both high density and viscosity ratios is incorporated to solve the Navier-Stokes equations. Also, unlike previous color-gradient models, the mobility is not related to the density field but instead a constant coefficient.

Two series of numerical tests are conducted to validate the accuracy and stability of the model, where we compare simulated results with available analytical and numerical solutions. In the first set, the interfacial evolution equations are assessed, while in the second set the hydrodynamic effects are taken into account.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 570

Symmetrizing multiphase flow equations for improved accuracy

Authors: Reza Haghani-Hassan-Abadi[1]; Hamidreza erfaniGahrooei[2]; James McClure[3]; eirik flekkøy[4]; Carl Fredrik Berg[5]

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When modeling multiphase fluid flows, the summation of the order parameters (or phase-field variables) is equal to unity. This order parameter equation can be used to reduce the number of flow equations by one. This reduction in the number of flow equations is always valid analytically. However, when it comes to numerical modeling, we observe that this reduction leads to different solution depending on which flow equation is removed. Such lack of symmetry is undesirable, and assumed to be a source of inaccuracy. To avoid that the numerical solutions depend on the choice of the reduced set of flow equation, we introduce and investigate solution techniques that preserves the full set of flow equations, thereby removing the lack of symmetry in the numerical solutions. Although we restrict our study to phase-field equations, we believe that the findings are more general.
Two commonly used phase-field equations, namely the Allen-Cahn and the Cahn-Hilliard equation, are solved based on the lattice Boltzmann method. Also, the hydrodynamic equations are also solved with the same method using a recently developed lattice Boltzmann model that can handle both high density and viscosity ratios fluids. In this study we compare the solutions using the reduced set of lattice Boltzmann equations with the solution using the full set of lattice Boltzmann equations. In general, the method solving the full set of equations is not ensuring that the sum of the phase-field variables equals unity. We have therefore also tested a method where this is ensured by an additional error correction step. Our results are compared in terms of accuracy and computational cost. The introduced methods have an additional computational cost, however, we observe improved accuracy at early times.

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MS17 / **571**

Thermodiffusion and thermo-osmosis in porous media

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When a temperature difference is applied over a porous medium soaked with a fluid mixture, two effects may be observed, a component separation (the Ludwig-Soret effect, thermodiffusion) [1,2] and a pressure difference due to thermo-osmosis [3,4]. In this work, we have studied both effects using nonequilibrium thermodynamics and molecular dynamics. We have derived expressions for the two characteristic parameters, the Soret coefficient and the thermo-osmotic coefficient in terms of phenomenological transport coefficients, and we show how they are related [5]. Numerical values for these coefficients were obtained for a two-component fluid in a porous matrix where both fluid and solid are Lennard-Jones/spline particles. We found that both effects depend strongly on the porosity of the medium and weakly on the interactions between the fluid components and the matrix. The Soret coefficient depends strongly on whether the fluid is sampled from inside the porous medium or from bulk phases outside, which must be considered in experimental measurements using packed columns. If we use an equimolar methane/decane mixture in the bulk as an example, the results for the Soret coefficient give that a temperature difference of 10 K will separate the mixture to about 49.5/50.5 and give no pressure difference. In a reservoir with 30 % porosity, the separation will be 49.8/50.2 whereas the pressure difference will be about 15 bar. Thermo-osmotic pressures with this order or magnitude have been observed in frost-heave experiments [6].
A detailed study of a two-component fluid in slit pores revealed that the thermo-osmotic effect was driven by a thermal Marangoni effect, by the gradient in a temperature dependent surface tension along the pore walls [7].

Participation:

In-Person

References:

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MS08 / 572

Exploring the Impact of Heterogeneity and Flow Rate on Mixing and Displacement of Miscible Phases in Porous Media

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Miscible phase flow in porous media plays a significant role in many natural and industrial processes, such as CO2 sequestration, aquifer salinization, and soil pollution. In these processes, a less dense and less viscous invading phase mixes with a more dense and more viscous defending phase at the interface between the two phases. The resulting mixture at the interface has an intermediate density and viscosity based on the mixing ratio of the phases. The invasion pattern is determined by the rate of mixing and displacement between the phases, which is influenced by the miscibility ratio, viscosity, and geometry of the phases. Most previous research on miscible multiphase flow has been conducted using 2D Hele-Shaw cells, in which a resident phase is displaced by an invading miscible phase introduced at the center of a circular plate. However, these studies do not account for the complexity of porous media structure at the pore scale, where the uneven advancement of the invading phase due to capillary or viscous forces is dominated by the heterogeneity of the porous structure. In this research, we will address the gap between the pore scale and volume scale by examining how the inner structure of the porous medium, or heterogeneity, leads to various mixing patterns for different inlet pressures and heterogeneity levels. We will use a low viscosity fluid invading and mixing with a high viscosity fluid in a 2D porous media at various flow rates and heterogeneity levels to investigate the impact on fingering patterns and displacement to mixing patterns. Our results will show that these variations in displacement to mixing have a unique signature at the Darcy scale as measured by flux measurements, demonstrating that the pore scale phenomenon for miscible phase flow in porous media can propagate to the Darcy scale.

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Poster / 573

The negative and positive effects of hot water injection into coal seam on CBM production

Author: Dong Zhou[1]

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The injection of hot water into coal seam has both negative and positive effects on the production of CBM (Coalbed Methane). In terms of the negative effect, when the water is entering the pore network in coal, the relative saturation and permeability of gas are reduced and lead to the water-lock phenomenon dominated by capillary force, which prevents the migration of CBM. In terms of the positive effect, the adsorbed CBM can be desorbed as the coal seam is heated, which increases the gas pressure, so as to improve the migration power and water displacement capacity of gas. In this study, the evolution law of the water regions and the gas regions distribution with the coal temperature and the two-phase fluid pressures during the hot water injecting into the pore network in coal was analyzed through numerical simulation, and the percolation transformation conditions of water region and gas region was clarified, so that the mechanism of negative and positive effects of hot water injection into coal seam on CBM production can be revealed. In the engineering of enhanced exploitation of CBM by injecting hot water into coal seams, the negative effect of CBM production was transformed into the positive effect by continuously increasing the coal seam temperature.

Participation:

In-Person

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Poster / 574

Wettability alteration of microfluidic devices using plasma and its influence on trapping mechanisms in geological reservoirs

Author: Viktor Gredičak[None]

Co-authors: Claire Douat [1]; Aneta Slodczyk [2]; Lionel Mercury ; Sophie Roman [3]

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To tackle climate change and help smoother energy transition, Carbon Capture, Utilization and Storage (CCUS) technologies are seen as a primary line of defense. Storing carbon dioxide (CO2) in geological formations appears to be a feasible solution, yet there are many unknowns concerning the dynamics and safety of the storage. One of the important CO2 storage mechanisms is solubility trapping, i.e. mass exchange at the interface between the CO2 and the resident fluid (usually

brine). Current Representative Elementary Volume (REV) models have difficulty resolving complex interplay between different parameters like wettability, pore size distribution, multiphase flow field, entrapment/remobilization, etc; which imposes a serious limitation for accurate description of mass transfer processes at large scale. To capture and understand the full physics of the problem, it is necessary to look at the scale of one or several pores, typically in micrometer order. Since there is a lack of data on the influence of micro-scale parameters, we have decided to study the influence of hydrodynamic conditions, geometry and wettability, to propose a new formulation for pore-scale mass transfer rates. With the help of microfluidics experiments and atmospheric/cold plasma, this study contributes to the understanding of the processes governing subsurface systems at the pore scale which is the key to improving the accuracy of modeling of transport phenomena at a large scale. Simple rectangular dead-end pore glass micromodels are deployed to imitate geological porous media as the material is inert, sturdy and allows direct visualization of the flow and transport mechanisms at the pore scale. These micromodels allow us to trap one fluid (CO2 or water) while the other is flowing, thus studying the coupling between flow and mass transfer at the fluid-fluid interface. Having micromodels of various wettability is still challenging, therefore we developed a new method based on the injection of a helium plasma jet in the micromodels to modify the surface properties of the microchannels to imitate different rock wettabilities encountered in nature. So far, we have successfully propagated the plasma jet through microchannels with a minimum cross-section of 250x100 μm covering the distance from the inlet to the outlet of 4 cm. As a result of treatment, the wettability of microchannel surfaces varies from moderately water-wet (contact angle ≈ 45°) to dominantly water-wet (contact angle ≈ 20°). We show that this wettability alteration can last for days in storage and several hours in experiments depending on experimental parameters. Moreover, we study the influence of wettability on the mass transfer rates following imbibition (dissolution of trapped CO2 bubbles in a stream of flowing water), and drainage (evaporation of water droplet in a stream of dry CO2) experiments by analyzing image sequences of the process for altered and non-altered micromodels. Our first results show that during imbibition the alteration of the wettability towards water-wet characteristics affects the trapping mechanism of CO2, while during drainage it influences the mass transfer rate. To explain and back up these results with statistical relevance, more experiments are being performed.

Participation:

In-Person

References:

Agaoglu et al., 2015;
Li et al., 2020;
Maes & Geiger, 2018;
Nernst, 1904

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Poster / 575

Understanding the Reactive Transport and Retention Behavior of Engineered Virus-mimicking Nanostructures

Authors: Jai Kishan Rajak[1]; Jan Willem Foppen[2]; Sulalit Bandyopadhyay[1]

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With the recent COVID-19 pandemic, different viruses in the environment and their disastrous effects has drawn the sharp attention of researchers and scientists worldwide. In recent years, the release of viruses has been a serious concern around the globe.
This inspired us to investigate more about what happens once a virus is released. Deciphering how various virus species act in a system of environmental mobility will be extremely interesting. This will enable us to understand and forecast their fate and transport behavior in various subsurface environments.
The release and migration of viruses in aqueous environments is a primary focus of this investigation. A short examination of the literature reveals that the majority of articles focus on representative viral species, such as bacteriophage MS2 and PhiX174. This might be an earlier made hypothesis on common viral behavior. Here, it is assumed that model viruses show similar transport and retention phenomena as all hazardous viruses. This might be due to various regulatory constraints and challenges that come into the picture when working with viruses that are lethal to humans. We assume that different viral species may behave differently based on their surface chemistry and physical morphology. Which has not been accounted distinctively in the literature, as most of them use model virus strains. Therefore here, we put out our hypothesis that natural viruses or more specifically their surfaces can be mimicked by utilizing engineered nanoparticles. Such surfaces can be further compared with natural viruses in terms of their transport and retention behavior in a saturated porous media environment.
Here, we are using a novel approach for synthesizing, surface-modified silica nanoparticles to closely resemble the physicochemical characteristics of virus surfaces. Physical characteristics like size, shape, and surface morphology are closely considered during the synthesis and post-modification processes, as well as surface chemistry characteristics including surface potential, particle density, and soft framework. These particle surficial features will be achieved in several stages of modification and optimization in the synthesis process. This will let us study the effect of individual elements on nanoparticle transport and retention behaviors. The results from the column sorption experiments will be studied under different environmental conditions and interpreted using numerical modelling tools.

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In-Person

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576

Assessment of the reversible degradation pathway of Diclofenac in soil-water systems

Authors: Laura Ceresa[1]; Alberto Guadagnini[1]; Giovanni Porta[1]; Monica Riva[1]

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Groundwater contamination by Pharmaceuticals is documented to threaten the integrity of natural ecosystems and human health. Here, we focus on the Non-Steroidal Anti-Inflammatory Drug *Diclofenac*, which poses critical concerns due to its continuous release and frequent detection worldwide. Experimental evidences yield controversial results on effective biodegradability of this molecule in groundwater, a peculiar behavior being observed under reducing redox conditions. In this context, batch microcosm experiments have revealed the occurrence of a reversible biotransformation pathway of Diclofenac in groundwater under biotic, denitrifying redox conditions. Such a behavior appears not to be captured by model formulations that are too streamlined, e.g., modeling approaches relying on first order reaction kinetics. In light of this, we suggest a modeling framework which is grounded on a conceptualization (and ensuing mathematical formulation) of the molecular dynamics of Diclofenac biodegradation in the considered scenario. We leverage on available laboratory-scale batch experiments associated with a soil-water system and embed the resulting model formulation in a stochastic context. We address the way the available information content can be effective in characterizing specific model processes upon (progressively) reducing the complexity of the proposed geochemical model. Four levels of simplification are considered in our study. The resulting mathematical formulations represent four plausible models. These are then employed in a multimodel context to interpret the considered system dynamics conditional to available data. Each candidate model is calibrated through a Maximum Likelihood approach assisted by modern sensitivity analyses techniques. This enables us to quantify the impact of model structure and parametric uncertainty on relevant model outputs, such as the temporal evolution of Diclofenac concentrations. The performance of each plausible model is then assessed (in a relative sense) through model discrimination criteria. Our results suggest that an optimal trade-off in terms of model complexity (i.e., level of parametrization) given data availability can be assessed to satisfactorily interpret the system dynamics.

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Poster / 577

Multiscale network modeling of flow in carbonate rocks with microporosity

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Diagenetic events lead to substantial variation in pore size, shape, and connectivity in carbonate rocks and porosity at multiple scales (submicron to hundreds of millimeters). This diversity in carbonate porous systems has a significant effect on petrophysical properties leading to different flow

characteristics in carbonates from that of siliciclastics. In this study, we focus on the role of microporosity (i.e., sub-resolution porosity) in multiphase flow through carbonate rocks with inherited structural and wettability heterogeneities. The study sample is a Ketton limestone (almost pure calcite) bearing a distinctly bimodal pore size distribution. The pore network of the Ketton sample is initially obtained using the generalized network extraction method, which allows three-dimensional (3D) pore space discretization of the underlying high-resolution X-ray computed microtomography (μCT) image (Raeini et al. 2017). In the generalized extraction workflow, all void space voxels in the μCT image are included in the network at different discretization levels. The resultant corners of the pore space extending from the throats at restriction points to the adjacent pore centers are identified as elements of the resolved network. In the network model created initially, only the resolvable macropores are considered (3.58 μm voxel size in our example). To characterize the sub-resolution porosity regions, differential imaging between μCT scan of the sample saturated with high-salinity brine as the contrast phase and dry scan is applied. This approach provides a porosity characterization based solely on interconnected porosity between macropores and sub-resolution micropores within grains, which contributes to flow and transport. The sub-resolution porosity regions are connected to the neighboring macro-porosity elements as equivalent effective links. In the flow simulations, the effective links representing microporosity networks do not undergo discrete pore-scale displacement events but are characterized by average pressure-saturation-conductance functions. The multiscale network model is calibrated with the Ketton carbonate macroscopic flow parameters measured by *in situ* μCT-monitored flow-through experiments under steady-state flow and altered wettability conditions (Zhang et al. 2022). The experimentally validated multiscale network model capturing sub-resolution pore space can be used for more quantitative future flow and transport studies in complex porous systems where the inclusion of microporosity yields more accurate predictions.

Participation:

In-Person

References:

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Zhang, G., Foroughi, S., Raeini, A.Q., Blunt, M.J. and Bijeljic, B., 2022. The impact of bimodal pore size distribution and wettability on relative permeability and capillary pressure in a microporous limestone with uncertainty quantification. Advances in Water Resources, 104352.

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MS04 / 578

Drying-induced bending of hydrogel disks

Authors: Jean-Francois Louf[1]; Haohui Zhang[2]; MaryKate Neff[3]; Yuhang Hu[2]; Sujit Datta[4]

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Hydrogel actuators are typically made of a bilayer gel that can promote water diffusion in one of the layers, subsequently inducing bending. Here, we show that similar bending behavior can be achieved by simply drying a hydrogel disk on a substrate. By varying the gel's aspect ratio and the substrate surface energy we are able to either observe (1) a deposit stuck to the substrate, (2) the bending of the hydrogel disk, or (3) planar drying until buckling of the disk occurs. This bending/buckling phenomenon is due to the coupled diffusion, deformation, and glass transition that freezes the deformation of the material elements in the hydrogel disk at different stressed states during evaporation. We further develop a finite element model to illustrate the role of the adhesion between the gel and the substrate in determining the different final shapes of the dried hydrogel disk. Together, our results provide both fundamental and application insights on, e.g., the drying-induced buckling of thin disks, an active field of research in the colloidal suspension community; and the design of new actuators, sensors, or even origami using differential drying.

Participation:

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Energy Transition Focused Abstracts:

MS01 / **579**

An image-based sphere insertion method for porous media drainage simulations with gravity

Author: Eric A. Chadwick[1]

Co-authors: Lukas H. Hammen [2]; Volker P. Schulz [2]; Aimy Bazylak [1]; Mario A. Ioannidis [3]; Jeff T. Gostick [3]

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Simulations of two-phase flow in porous media are of interest in a wide range of fields such as groundwater remediation, oil and gas extraction, and hydrogen storage devices [1–5]. In the field of hydrogen storage, the flow of gases and liquids in porous media layers of fuel cells greatly impact their performance [6]. Historically, continuum models have been the most prominent as they are useful for observing macroscopic phenomena, such as flow in deformable porous media or in electrochemical devices [7–10]. However, continuum methods do not lend themselves to investigating pore-scale phenomena in two-phase flow. Moreover, pore-scale simulations typically neglect gravity as it is assumed that the pores are small enough that capillary forces are dominant over gravitational forces [11,12]. In this study, we present our adaptation of the established full morphology method

[1,2] that allows for the inclusion of gravitational forces during drainage simulations. Unlike traditional full morphology methods, our method does not rely on morphological image processes but rather utilizes calculated image-based sphere insertion (IBSI) to simulate an invading non-wetting phase.
To include the effect of gravity in the IBSI approach, we utilized a distance transform approach with two modifications. In previous studies that use the standard approach without gravity, a distance transform was used to determine the radius of a meniscus that can fit at each pixel of the pore space [1,2]. One key step for incorporating the effect of gravity was to convert the values of the distance transform to reflect their vertical distance from the inlet. This requires converting the distance values to a capillary pressure using the Young-Laplace equation, assuming the two interacting fluids are fully non-wetting and the interface is spherical in shape. Then, the pressure in each voxel was calculated based on their respective heights. A seed voxel was then placed at all locations of non-solid space in the image where the pressure was lower than the applied inlet pressure. Finally, to simulate the advancing meniscus, spheres were placed at the center of each seed point with a radius determined by the initial distance transform.
The IBSI method was validated using capillary tubes demonstrating a mean error of 1.83 ± 5.45 % compared to analytical solutions and further compared to experimental values from literature [13]. Simulations on 2D and 3D stochastically generated porous media were performed to demonstrate the impact of neglecting the effects of gravity in drainage simulations in the generated porous media. The absolute saturation error, defined as the difference between the saturation with and without the consideration of gravity, increases as the Bond number and the height of the porous media domain increases, as shown in the contour plot below. Through these results, it was shown that gravity can play a significant role in drainage at low bond numbers («1), especially in large domains (>10 mm in height). It is therefore recommended that gravity be considered when studying drainage in porous media domains at the centimeter or greater scale such as in large-scale fuel cell stacks.

Participation:

In-Person

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581

Hydrogen storage in a water-filled 2.5D micromodel

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The use of hydrogen as a source of energy has recently gained attention. To meet the growing demand for hydrogen, it is essential to build reliable large-scale hydrogen storage capacities. Underground geological formations such as aquifers can provide a feasible solution for storage. Hydrogen interactions with in-situ fluids in reservoirs, permeation through porous rock, and reproduction to the surface should be understood to design an underground storage facility in depleted reservoirs. While numerous studies have focused on different aspects of underground hydrogen storage, there is a lack of understanding regarding the impact of rock-fluid properties on the interactions between hydrogen and water at the pore level.

In this study, we investigate the effect of water salinity on the micro-scale hydrogen-water interactions during the drainage and imbibition processes. The experiments are performed using a 2.5D borosilicate micro model. The micro model is designed to have high-permeable horizontal channels which are connected with low-permeable zones. In the drainage experiments (hydrogen storage), water is produced at a constant rate of 5 µl/min while the hydrogen pressure at the inlet is kept constant as 11.3 psi. Images of water drainage process shows that hydrogen initially sweeps the high permeable channels and then jumps over the next high permeable channel by sweeping a few smaller pores. However, due to the imperfect occurrence of this phenomenon, residual water fingers are observed in high-permeable pores. This process continues until the breakthrough time while no changes in the system is recorded after the breakthrough during the hydrogen injection. The process is reversed to imbibition (hydrogen production) by water injection at a constant rate of 5 µl/min and keeping the hydrogen pressure constant at 11.3 psi. During the imbibition process, the advancement of the main water-hydrogen front is not evident while we record the formation of isolated snap-offs throughout the micromodels. This phenomenon originates from the advancement of corner flow which results in the trapping of hydrogen in large pores. Hence, the displacement efficiency and the hydrogen storage capacity are reduced. The impact of water salinity on the drainage and imbibition cycles is analyzed by adding salt (NaCl) at 2000, 20000, and 200000 ppm to the water phase. All salt concentrations exhibit similar overall fluid distribution to what we observed in DI water. However, the number and total length of residual water fingers are found to be decreasing functions of water salinity. We speculate that the salt effect could be due to an increase in the interfacial tension between hydrogen and water at higher salinities. The present experiments demonstrate that hydrogen storage in the designed pore-network model increases by salinity primarily due to the lower volume of residual water fingers at higher salinities. However, the stronger capillary forces in the higher salinity cases intensify the corner flow which leads to lower volumes of displaced hydrogen. These two effects balance out the volume of recoverable hydrogen in all scenarios. Thus,

despite the differences during the drainage and imbibition process, the storage capacity is similar in all salinities.

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583

Droplet dynamics at the interface between gas diffusion layer and gas distributor channel in polymer electrolyte membrane fuel cells

Authors: Maziar Veyskarami[None]; Rainer Helmig[1]; Carina Bringedal[None]

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In a polymer electrolyte membrane (PEM) fuel cell, the interaction between the gas distributor channel (GDC) and gas diffusion layer (GDL) is of great importance. Emerging of water droplet on the interface between GDL and GDC, especially at the cathode side, significantly alters mass, momentum and energy exchange between the two domains. In order to capture such impacts, we developed a model consisting of a porous medium, GDL, which is coupled with a free flow channel, GDC. To describe the porous medium, we use a pore network model developed by [1, 2]. The Navier-Stokes equations describe the flow in the free flow domain. New sets of coupling conditions between the domains are derived, which take the droplet impact into account. A concept is developed to include droplet dynamics at the interface such as formation, growth and, finally, detachment of the droplet due to the free flow. Here, we discuss the model development and compare the simulation results of the model with experimental data. In addition to helping us to gain a better understanding of the droplet formation at the interface between GDL and GDC, our model could provide a basis for further developments.
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Participation:

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References:

1 Weishaupt, K., Terzis, A., Zarikos, I., Yang, G., Flemisch, B., de Winter, D. A. M., & Helmig, R. (2020). A Hybrid-Dimensional Coupled Pore-Network/Free-Flow Model Including Pore-Scale Slip and Its Application to a Micromodel Experiment. Transport in Porous Media, 135(1), 243–270.
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Rapid modeling of deep learning surrogate based models for CO2 utilization and sequestration

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Carbon dioxide utilization and sequestration, as one of the principal means of carbon burial, provides an economic and feasible technological means to mitigate global warming. In order to utilize CO_2 optimally and reduce the risk of leakage, a large number of numerical simulation processes are required for multiphase flow in porous media.Efficient and speedy numerical simulation of inhomogeneous multiphase flows can greatly increase resource utilization and economic benefits, in addition to supplying timely and reliable technical guidance for subsequent optimization measures. Moreover, as a result of the inherent inhomogeneity of strati graphic porous media and the nonlinear coupling of multiple complex physical processes, the numerical simulation process of multiphase flow incurs significant computational costs and requirements a lot of time to implement.And with simulation cost and computation time constraints, it is frequently challenging to complete high-fidelity flow numerical simulation modeling speedily.
As an effective complement or alternative to the original model, the surrogate model offers the potential to accelerate the modeling of complex models without the sacrifice of accuracy or detail, as opposed to the flow numerical simulation modeling process. In this work, we develop a rapid and efficient deep learning-based surrogate modeling workflow to provide accurate and efficient predictions of formation CO_2 utilization and storage processes.Instead of designing neural network architectures exclusively for a specific porous medium flow problem, we incorporate neural network architectures and loss functions into the surrogate model optimization process with several neural network architectures as alternatives and set up loss functions with variable parameters in reference to the design of loss functions used in image restoration work. In purpose of rapidly optimizing the surrogate model, this study establishes a target-specific objective function to characterize the prediction effect of the surrogate model under different parameter combinations. Following the consistent objective function, we established a complete surrogate model optimization process which is based on the TPE (Tree-structured Parzen Estimator) algorithm. We have set up a carbon dioxide storage in brackish water layer case and a carbon dioxide oil drive case, based on the workflow proposed in this study to construct a surrogate model using simulated flow simulation data. In the above case, the surrogate model achieved accurate predictions for 120 time steps with different production parameters, formation parameter distributions and well placements, and its average relative error in predicting pressure and saturation plume on the test set was 0.241% and 0.254% respectively, with

mean structural similarity index (SSIM)of 0.9987 and 0.9998 respectively. Therefore, the workflow proposed in this study has a relatively high adaptability and effectiveness, and can be expected to contribute to the development of CO_2 utilization and storage.

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Poster / 586

Hydraulic attributes of heterogeneous pore spaces

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We design porous geometries with different grain organizations and embed these in novel microfluidics set-ups to directly assess hydraulic attributes of porous media as a function of the degree of structural complexity of the pore space. A variety of studies have documented the relationship between the overall flow and pressure drops for homogeneous permeable media. Otherwise, the fundamental nature of such a relationship within heterogeneous system characterized by a broad range and a complex arrangement of pore sizes is still not completely explored. Here, we couple microfluidics experiments and direct observation of (a) flow through the designed geometries while imposing a macroscopic pressure gradient as well as (b) flow patterns therein with detailed numerical simulation of flow. We the synthesize the results upon deriving an analytical formulation relating the overall intrinsic permeability and key features of the porous structure. While our formulation is grounded on the classical Kozeny-Carman relationship, it embeds the spatial variability of pore sizes, thus contributing to enhance our knowledge on the feedbacks between the microstructure of the pore space and the overall medium permeability.

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587

A New Hybrid Pore-Scale Simulation Method to Characterize Nanoparticles Transport and Attachment Behaviors in a Microchannel

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To promote the applications of nanoparticles (NP) for various subsurface reservoir engineering, it is fundamental to characterize the transport and attachment behaviors of NPs in microscopic scale. A novel, hybrid pore-scale simulation method using Lattice-Boltzmann (LB) coupled with Langevin-Dynamics (LD) is proposed to investigate the transport physics of nanoparticles in microchannel. LD method is developed to characterize the physics of Brownian motion, thermal fluctuation dissipation, multi-body hydrodynamics and particle-particle interactions. A discrete LB forcing source distribution is employed to couple with LD. Random force of NPs, friction force of NPs, van der Waals force and electrostatic force between NPs and the microchannel are quantified in this Euler-Lagrange method, in order to more accurately simulate the transport and attachment process of NPs. A variety of examples (i.e. single particle relaxation in viscous flow, Brownian motion in the dilute colloid system, the attachment efficiency of NPs onto channel surface) are implemented to verify the LB-LD method. The controlling factors (i.e., ionic strength, particle diameter and Reynolds number) are investigated in the attachment process of NPs. The NP with intense Brownian diffusion and weak hydrodynamic effect are prone to have better attachment efficiency. It is observed that a threshold value of attachment efficiency exists as the ionic strength increases to about 0.01 M. Moreover, the ionic strength of aqueous phase has critical effect on the transport behavior of NPs: when the ionic strength is less than 0.005 M, an ordered structure of NP suspensions is obtained due to the dominance of electrostatic repulsion force; Varying structures of NP suspension are observed with the increase of ionic strength; as the ionic strength is more than 0.01 M, a clustered structure of NP suspensions is derived by the dominance of van der Waals force. For the purpose of quantitatively characterizing the structure of NP suspensions under varying conditions, a general phase diagram including three flow patterns (isolated, transitional and clustered regime) is first proposed for NP suspension with specified ionic strength and Reynolds number. The outcomes of this work provide valuable insight on the critical importance of the particle size, ionic strength and hydrodynamic effects on the attachment and transport process of NPs in porous media.

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Poster / 588

Influence of Pyrolysis Residence Time on The Physicochemical Properties of Algal Biochar for Water Treatment

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Access to clean water have been a growing problem for both developed and underdeveloped countries. To curtail this growing problem, water treatment must be considered. Conventional methods such as chemical precipitation, ion exchange, adsorption (using activated carbon), and membrane separation processes are applied in the removal of contaminants from water. These methods are costly and often generate considerable amounts of chemical residues, which have no economic value. Biochar derived from the pyrolysis of various biomass has shown to be a promising material for water treatment. Biochar can be produced from a wide range of feedstock including plant and animal wastes, domestic and municipal wastes, agricultural waste, and more recently algae (seaweed).
The influence of pyrolysis temperature on the physiochemical properties of biochar has been studied and well established (Frota et al., 2022, Wang et al., 2020). In contrast, less attention has been paid to the effect of the residence time on these physicochemical properties.
This work is focused on the impact of pyrolysis residence time on surface and chemical properties of Ulva rigida algal biochar (URB). Residence times of 15min, 30min, 45min, 1hr, 1hr:30min and 2hr, and at a fixed temperature of 600oC. We studied the Ulva rigida (UR) algae which is a seaweed that thrives in polluted shallow worldwide.
We aim to understand the influence of above residence times on the surface and chemical properties of the algal biochar such as composition, morphology, crystallinity, surface area, pore size distribution, change in aromaticity and polarity by TGA/DSC, SEM, EDX, XRD, BET and FTIR measurements.
As earlier reported by other researchers increased residence time had significant effect on biochar physicochemical properties. It was found to increase the surface area, porosity, pH, and ash contents of biochar but decreased C, N and H contents. Prolonged residence time resulted in collapse of pore structure and decreased surface area (Sun et al., 2017, Wang et al., 2020).
This study would investigate if the above pattern of surface and chemical properties will be retained by Ulva Ridiga biochar (URB) which will aid in our future studies such as biochar selection, process time and pyrolysis temperature optimization for a better material design of water treatment.

Participation:

In-Person

References:

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Accurate and fast rock image segmentation using U-net with a Mobile-net backbone

Authors: Marzieh Ghadimi Mahanipour[None]; Mohammad Emami Niri[1]

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Segmentation of grey micro CT images plays an essential role in any digital rock physics workflow. As user bias and subjectivity were often recognized as a drawback of the traditional segmentation methods, developing an automated system have always been proposed. Deep learning methods have attracted many researchers'attention to use them in digital rock physics (including segmentation) and the results were often successful. Despite the high accuracy, the neural networks suffer from high computational time and huge memory requirements, especially for large input images which in the energy industry is not so critical as medical emergencies where fast processing using devices with limited memory is required to make the quick right decision, for example during a surgical operation. That is why accelerating neural network training and inference has been untouched by digital rock physics researchers. But what if one could take a photo of drilling cuttings with his cell phone, reconstruct it to a high resolution then segment and calculate its properties even dynamic ones like permeability. One of the prerequisites to achieving this goal is reducing the networks' number of parameters.

Among different neural networks, U-net has been extensively used in rock segmentation. It involves an encoder-decoder structure with skip connections. Since it was first introduced in 2015, several modifications to its architecture have been proposed. One of them is replacing the encoder part with well-designed classification networks like Res-net, Efficient-net, VGG16, Inception, Mobile-net, etc. The encoder could be loaded using weights obtained by training on data sets like image net and then only the decoder needs to be trained. Mobile-net with depth-wise separable convolutions is a lightweight neural network that causes speed up in both training and inference time.

In this study, we used U-net with a Mobile-net backbone for a three-phase rock segmentation. We applied the segmentation models library which was created using Keras and TensorFlow frameworks. Image patches of size 96×96 which are extracted from a North Sea sandstone image (6,100 × 6,100 pixels) by sliding a window are used for network training. More representative segmentation losses (Jaccard, Dice, Focal) and metrics (IoU, F-score) are employed which prevent misinterpretation about the quality of segmentation against pixel accuracy. Our results show using Mobile-net against Efficient-net as the backbone of a U-net resulted in a 2-4 times decrease in both training time and the number of parameters without loss of accuracy.

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Energy Transition Focused Abstracts:

MS21 / 590

Dynamics of $A + B \rightarrow C$ chemical reaction fronts in finite radial geometry

Author: Darío M. Escala[1]

Co-authors: Anne De Wit [2]; Fabian Brau [1]

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Transport of species in porous media plays a crucial role in a variety of fields, including environmental engineering, geochemistry, and biology. Understanding the movement of species such as contaminants, nutrients, and microorganisms through porous media is essential for predicting and mitigating the impacts of human activities on the environment, as well as for developing effective remediation strategies 1. For example, in the field of environmental engineering, knowledge of species transport in porous materials is essential for designing effective remediation strategies for contaminated soil and groundwater. In other applications such as water treatment, understanding the transport of nutrients and contaminants in porous media can help in the design of filtration systems and the optimization of treatment processes [2]. Additionally, research on transport of CO_2 in porous media is crucial for developing and implementing effective strategies for carbon sequestration in aquifers, which is a key component of efforts to mitigate climate change [3]. In general terms, the study of transport of species in porous media has the potential to significantly improve the effectiveness and efficiency of a wide range of environmental and engineering technologies.
In this study, we investigate the behavior of $A + B \rightarrow C$ reaction-diffusion chemical fronts in a finite radial geometry where the chemical species A and B are initially separated in space. In addition to the time properties found for rectilinear ([4]-[6]), and radial ([7]) geometries, we describe the dynamics of the spatial position of the reaction front (AB) which strongly depends on the initial parameters such as the ratio of initial concentrations ($\gamma = B_0/A_0$), ratio of diffusion coefficients ($\delta = D_B/D_A$), and the size of the geometry (R). We performed simulations and numerical analysis to predict the dynamics of the front and compared our results to experimental observations performed in gel and liquid systems.
Unlike previous studies done in infinitely extended domains, our results show that the reaction front could remain stationary at any spatial position depending only on the initial conditions. With the aforementioned numerical analysis, we are able to predict the short, medium, and long-time dynamics of the reaction front.
Our findings provide new insights into the behavior of $A + B \rightarrow C$ chemical fronts in finite radial geometry. By better understanding these dynamics, we can improve our ability to control and manipulate chemical reactions in more complex settings.

Participation:

In-Person

References:

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Relaxation modeling for convection-diffusion problems

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We propose a new relaxation modeling applied to partial differential equations with convective and diffusive terms. We recast the underlying convection-diffusion problem into a coupled system of hyperbolic equations with relaxation terms. In contrast to the previous related relaxation modeling results in the existing literature, where the solution of the reformulated problem converges to some type of equations in the diffusive limit, here, in our formalism, the augmented problem is treated as coupled hyperbolic equations with a relaxation acting in both, the purely convective flux and the source term. Indeed, we also show that the new system of equations satisfies Liu's sub-characteristic condition. We perform numerical experiments to several important models, including a nonlinear convection-diffusion problem with discontinuous coefficient, aiming to verify the robustness of the proposed approach, evidencing that this relaxation modeling is promising and it can be applied for relevant problems in pure and applied mathematical sciences.

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Energy Transition Focused Abstracts:

MS01 / **592**

Impact of microbial activity on hydrogen transport in porous reservoirs across scales

Author: Maartje Boon[1]

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Geological porous reservoirs are seen as an attractive solution for large scale underground hydrogen storage (UHS). Microbes are expected to be abundant in these reservoirs and could have a significant impact on the UHS process as the stored hydrogen can be used in their metabolism. Next to adverse effects such as hydrogen loss, H2S formation and clogging, microbial activity could alter the wettability of the hydrogen/brine/rock system and, consequently, the hydrogen transport behavior during UHS.
To effectively exploit these reservoirs for UHS, a good understanding of the impact of microbial activity on the hydrogen transport behavior inside porous rock is crucial. In this work, we characterize hydrogen transport properties in a microbial active environment from the pore- to the core-scale using several experimental techniques: Wettability is characterized using the captive-bubble cell approach and microfluidics, while relative permeability and capillary pressure are measured during core-flood tests at the core-scale. The activity of the living brine used in the experiments, which contains the sulphate reducing bacteria "*Oleidesulfovibrio alaskensis*"is continuously monitored through the pH. Our preliminary results show that high microbial activity increases the contact angle with around 5°, making the hydrogen/brine/rock system less water-wet.

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MS06-A / 593

Upscaled model for two-phase flow in porous media

Author: Didier Lasseux[1]

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The formal derivation of the macroscopic mass and momentum balance equations for two-phase, creeping incompressible and Newtonian flow in rigid and homogeneous porous media is proposed in this work, assuming separation of length-scales and the existence of a (periodic) representative elementary volume, both classical for upscaling. The development is performed by making use of elements of the volume averaging method, combined with the adjoint technique and a Green's integral formulation [1, 2]. The macroscopic mass balance equation in each phase is identical to that already reported in the literature [3, 4]. The macroscopic momentum balance equation expresses the seepage velocity in each phase under the form of a pair of Darcy-like terms, involving a dominant and coupling permeability tensor, respectively related to viscous effects in the phase under concern and viscous coupling through the interfaces. Importantly, it includes an additional term resulting from capillary effects. The later has not been obtained so far as a result of a priori assumptions that this term should be negligible, in particular for small capillary numbers [4, 5, 6]. The effective coefficients present in this macroscopic model are all obtained from the solution of two coupled closure problems that coincide with those already reported in the literature [4, 5, 6, 7]. The performance of the model is illustrated with numerical simulations carried out in a model two-dimensional configuration using a boundary element method. Average velocities, resulting from direct numerical simulation, are compared to the predictions of the macroscopic model obtained from the closure problems solution, showing excellent agreement over extended ranges of the capillary number, viscosity ratio and wetting-phase saturation. The additional capillary term present in the average momentum equation is shown to have a very important contribution is some situations. Extensions to other flow situations are briefly discussed.

Participation:

In-Person

References:

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MS10 / 595

Multiscale analysis of microporosity of deep marine reservoir rocks using hard X-rays zoom microtomography of synchrotron source

Authors: Daphne Silva Pino[1]; Paola Cunha Ferraz[2]; Allan da Silva Pinto[1]; Larissa Macul Moreno[1]; Bruno Vasco de Paula Carlos[1]; Otávio Moreira Paiano[1]; Eduardo Xavier Miqueles[1]; Rodrigo Surmas[3]; Nathaly Lopes Archilha[4]

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The pre-salt is a geological formation of sedimentary rocks with organic content formed more than 100 million years ago, by the accumulation of organic matter on the south-eastern coast of Brazil during the separation of the American and African continents. The subsequent formation of the Atlantic Ocean led to the subsequent deposition of a layer of salt, which nowadays reaches 2 km in thickness. The salt layer was responsible for trapping the organic content, enabling thermochemical processes that generated oil and natural gas in the pre-salt layer. The latter is currently located 5 km deep below sea level.

The goal is to study the microporosity of reservoir pre-salt rocks in multiple scales using hard X-ray (39 keV) zoom microtomography, at the MOGNO beamline at the Brazilian Synchrotron Light Laboratory. MOGNO's conic beam allows image acquisitions with different pixel sizes by varying the sample position relative to the source and the detector, also enabling the user to image relatively large samples.

Preliminary tests were performed with pre-salt rock plugs of 3 mm diameter. The sample was positioned along the beamline for the acquisition of images at four resolutions, with 2.0, 1.5, 1.0 and 0.5 μm pixel sizes. Different algorithms for image reconstruction and segmentation are currently being studied. The former includes FDK (Feldkamp, Davis and Kress) and EM (Expectation Maximization) algorithms. The latter comprises methods of supervised and unsupervised machine learning algorithms based on image texture.

We expect to be able to correlate micropores and pores throughout the different scales and, by future analysis of other pre-salt reservoir rocks with zoom XR-μCT, to shed light into petrophysical models for a more efficient oil exploitation.

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References:

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596

Estimation of mineral accessible surface area from mineral abundance and clay content

Authors: Md Fahim Salek[1]; Fanqi Qin[None]

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Variation in mineral reactive surface area measured through various approaches (e.g., Brunner-Emmett-teller adsorption, geometry approximation, imaging techniques) results in large discrepancies in simulated geochemical reaction rates. Recent studies have shown that simulations carried out using mineral accessible surface areas (ASAs) estimated from coupled 2D and 3D imaging better reflect the observed reaction rates measured in core-flood experiments. However, image processing is both time and resource-consuming. In this work, the possibility of estimating mineral ASAs from easily measured properties like mineral abundance and porosity is explored. Sandstone samples from six different formations were studied, along with data obtained for three additional samples from previous literature. Samples were imaged in 3D and combined with data obtained from 2D mineral segmented maps to quantify mineral ASAs. Sample properties like porosity, mineralogy, mineral accessibility, and ASAs were compared to explore potential correlations between them. The results show that accessibility of quartz, K-feldspar, and albite minerals can be estimated based on knowledge of the overall mineral composition; while feldspar mineral accessibility generally increases with increasing abundance, quartz accessibility decreases with increasing clay content. Mineral ASAs vary between samples, depending on the relative abundance of minerals and overall pore connectivity. ASA of quartz decreases with abundance; on the other hand, albite and carbonate mineral ASAs increase with abundance. This approach may largely reduce the required extent of image analysis where ASAs could then be quantified simply from mineral composition quantified from other methods such as XRD. Additional samples need to be considered for meaningful observations of different mineral phases.

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MS03 / 597

Groundwater Model Development of a Fractured Crystalline Rock Site with Site-Specific Data

Authors: Stefano Normani[1]; Andrew Snowdon[1]; Eric Sykes[2]; Aaron DesRoches[2]; Andrew Parmenter[3]; Jonathan Sykes[1]

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A site selection process is currently underway in Canada to select a site for a deep geologic repository (DGR) for Canada's used nuclear fuel. Currently, two potential siting areas are undergoing evaluation: one in plutonic crystalline rock in the Canadian Shield, and one in sedimentary rock. The focus of this study is the crystalline site. As part of ongoing site investigation activities, Canada's Nuclear Waste Management Organization (NWMO) has drilled and instrumented multiple kilometre-long, vertical and near vertical, boreholes. Extensive data has been collected from in-situ borehole geophysical and hydraulic testing, opportunistic groundwater sampling, and in-situ borehole fluid pressure measurements. The influence of increasing fluid density is evident in the equivalent freshwater head estimations.

The Canadian Shield is composed of fractured Precambrian rock that is known to have high total dissolved solids concentrations (TDS), in some cases exceeding 300 g/L. The high TDS values observed in the Shield affect fluid density, resulting in the coupling of the groundwater flow equation with the solute transport equation for TDS. In this study, numerical groundwater models are developed as a means to assemble and integrate site-specific data and illustrate the evolution of flow and salinity transport at the site over geologic time. A three-dimensional finite-element groundwater model mesh covering an area of approximately 400 km^2 was developed. Model boundaries were selected to correspond with surface water divides and assumed groundwater divides. The numerical groundwater modelling is being performed using HydroGeoSphere, a computational model that includes both porous media and discrete fracture zones. Deterministic inferred fracture zones delineated from surface lineament features with trace lengths greater than 500m were generated using GoCAD. FracMan was used to generate stochastic Discrete Fracture Zones (DFZs) ranging from 100m to 500m in equivalent length for a site-scale domain. These discrete fracture zone networks are conditioned to a comprehensive borehole and rock core fracture data set and embedded within the regional scale three-dimensional hexahedral finite element mesh. Orthogonal fracture faces, between adjacent finite element blocks, were used to best represent the discrete-fracture zone networks. Discrete fractures with an equivalent length of less than 100m are included in the equivalent porous medium (EPM) rock mass.

Model parameterization includes depth-dependent hydraulic conductivity and transmissivity profiles for both the EPM rock mass and fracture zones, based on in-situ borehole hydraulic testing data. A correlated Gaussian random field is used to designate portions of fracture zones as either open (33%) or closed (67%), with the partitioning corresponding to conservative assumptions based

on borehole core logging and available hydrogeological data. The open portions are parameterized using mean depth-dependent fracture zone transmissivity values. Lab estimated values of porosity are corrected for estimated in-situ stress. Hydraulic estimates from packer tests are used to condition the permeability of the EPM rock mass and fracture zone transmissivity. A first-order source term for brine is applied to account for the in-situ evolution of TDS based on rock-water interaction over hundreds of millions of years. Density-dependent groundwater flow, solute transport, groundwater age, and mean time to discharge simulations are demonstrated.

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Energy Transition Focused Abstracts:

598

Lattice Boltzmann Simulation on Reactive Transport of Calcite Dissolution by Injecting CO2-saturated Brine during Sequestration

Author: Qiuheng Xie[1]

Co-authors: Wendong Wang [1]; Yuliang Su [1]; Sina Rezaei-Gomari [2]; Han Wang [1]; Zhouyuan Zhang [1]; Wubin Yan [1]

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CO2 as a kind of greenhouse gas has a greatly adverse impact on the environment, and fixing carbon into saline aquifers effectively alleviates the effect it brings. In the present study, the calcite dissolution during sequestration near wellbores at different temperatures is explored to elucidate the mesoscale mechanism of reaction transport during this process and the evaluation of hydraulic properties with time that affects the injectivity of CO2-saturated brine.

A multi-component lattice Boltzmann method coupled fluid flow, mass transport, heterogeneous reaction, and structure evolution is proposed to quantitively study the reaction transport of calcite dissolution near wellbores. A special solution included the general lattice Boltzmann concentration boundary condition and Volume of Pixel method is utilized to model the dissolution reaction. The influence of temperature on reaction dynamics in porous media is analyzed by exerting the Arrhenius expression, and the concentration distribution of H+ and Ca2+ is captured to reflect the dissolution front directly. Moreover, the evaluated hydraulic properties characterize the effect of the dissolution reaction on the brine injectivity.

Since the reaction rate of calcite dissolution increases with temperature, the dissolution node of calcite is proportional to the temperature at a constant pressure difference. And the dissolution node indicating the released volume of Ca2+ which is a key reactant for the mineral trapping is summed to estimate the sequestration result. Furthermore, the dissolution front observed from the pore-scale

simulation is heterogenous due to a higher velocity, and the dissolution pattern of all cases is identified as the wormholing dissolution, which means that the increasing porosity during the calcite dissolution has a great contribution to the permeability. Admittedly, the increasing temperature during sequestration is conducive to calcite dissolution and changes in hydraulic properties. For sequestration operation, the high-temperature formation is recommended for both the injectivity and the subsequent mineral trapping.
This work provides theoretical and pragmatic guidance to operators to design CO2-saturated brine injection in saline aquifers. Furthermore, the results can also promote cognition of the calcite dissolution for sequestration at different temperatures.

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Energy Transition Focused Abstracts:

Poster / 599

Laboratory measurements of fluid pressure diffusion in a fractured carbonate sample

Authors: Samuel Chapman[1]; Simon Lissa[2]; Jerome Fortin[1]; Beatriz Quintal[3]

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Better understanding the complex poromechanics of fluid-saturated fractured rock is important to numerous areas in the exploitation of subsurface resources. Fluid pressure diffusion (FPD) between fractures and the embedding porous matrix and/or between interconnected fractures can be a significant source of intrinsic seismic wave attenuation and dispersion, as indicated by theoretical studies (e.g. Brajanovski et al., 2005, Rubino et al., 2013, Quintal et al., 2019). Experiments investigating fractured rocks are scarce and only recently has FPD from a saw cut fracture into the porous matrix been demonstrated during hydrostatic oscillations of the confining pressure (Gallagher et al., 2022).

We extend the investigation of Gallagher et al. (2022) to a more realistic scenario by using a carbonate sample with naturally occurring fractures that were delineated with micro-X-ray computed tomography (CT). In a novel setup, two pressure transducers were implemented to probe the pore fluid pressure response in the main fracture and in the porous background. Strain gauges mounted on the surface of the sample measured the radial and axial strains of the porous sample. Ultrasonic P- and S-wave travel times were measured along the axis of the cylindrical sample and perpendicular to the interface of the main fracture. Hydrostatic confining pressure oscillations were performed on the glycerin saturated sample to investigate the bulk modulus dispersion and attenuation. By adjusting the temperature of the experiment (19 to 45 ℃), an apparent frequency range as broad as

4⊠10-3 to 7 Hz could be investigated by scaling the measured frequency with the change in glycerin viscosity. The sample, fracture, sensor configuration, the locally measured attenuation and bulk modulus dispersion, as well as the pore pressure are shown in the supplementary figure.

The dry sample had significantly higher P-wave velocities in the axial direction compared to that in the transverse direction. Increasing the confining pressure up to 17 MPa increased the P-wave velocities, but it did not impact the anisotropy. This observation suggests that small cracks in porous matrix were closed, while the main fracture remained partially open. In the glycerin saturated sample, we observed negative bulk modulus dispersion and attenuation, which is a consequence of measuring the strain locally on the sample surface with strain gauges, as numerically demonstrated by Chapman and Quintal (2018). At low frequencies the pore pressure is equilibrated between the fracture and porous matrix, but with increasing frequency we observed a higher pore pressure response in the matrix than in the fracture. A larger pore pressure response in the fracture was expected, due to its presumably larger compliance than that of the porous matrix. This unusual observation may be attributed to the large aperture of the main fracture in certain places where it potentially acts as a dead volume into which fluid can be drained from the other portions of the sample. The results highlight the complexity of the poromechanics of highly heterogenous and fractured rocks.

Participation:

In-Person

References:

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MS12 / 600

Seismic wave attenuation and dispersion due to two-phase fluid saturation: Laboratory measurements and numerical simulations based on X-Ray CT

Authors: Samuel Chapman[1]; Jan V. M. Borgomano[2]; Beatriz Quintal[3]; Sally Benson[4]; Jerome Fortin[1]

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The integration of poromechanical experiments under X-ray computed tomography with numerical simulations could improve the modeling of intrinsic attenuation of seismic waves by fluid pressure diffusion (FPD). This could lead to improvements in the monitoring of carbon dioxide storage sites where the sensitivity of the attenuation of seismic waves by FPD to the saturation and spatial distribution of the fluids could be used to assess residual trapping in a storage formation. However, this requires validating models of FPD with accurate measurements of seismic wave attenuation and modulus dispersion over a broad frequency range, as well as, parameterizing the fluid distribution during experiments.

Experiments were performed on a Berea sandstone sample where CO2 was allowed to exsolve from water following a reduction in pore pressure. The fluid distribution was determined with X-ray computed tomography (CT) in a first set of experiments. The CO2 exsolved predominantly near the outlet, resulting in a heterogeneous fluid distribution along the sample length. In a second set of experiments, at comparable pressure and temperature conditions, we investigated the attenuation and modulus dispersion in the partially saturated sample over a broad frequency range (0.1 - 1000 Hz) by applying force axial oscillations and measuring the stress-strain response of the sample. We observed significant attenuation and dispersion in the extensional and bulk deformation modes, with the Young's and Bulk modulus falling between the low frequency Gassmann-Wood limit and the high frequency Gassmann-Hill limit. No frequency dependent attenuation and dispersion was observed in the shear modulus. These observations are consistent with FPD at the mesoscopic scale in a mechanically isotropic rock.

The attenuation and dispersion by FPD were subsequently modelled by solving Biot's quasi-static equations of poroelasticity with the finite element method. The fluid saturation distribution determined from the X-ray CT was used in combination with a Reuss average to define a single-phase effective fluid bulk modulus. The numerical solutions agree well with the attenuation and modulus dispersion measured in the laboratory. The approach can be extended to include sub-core scale porosity and permeability distributions, which can also be determined from multiphase core flooding experiments in combination with X-ray CT. In the future this could allow for conducting experiments on heterogenous samples and accurately relating fluid distribution to the attenuation of seismic waves. Such an advancement will however require the development of a new experimental setup capable of measuring the quasi-static stress-strain response of samples concurrently with X-ray CT.

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Poster / 601

Pore-scale simulation of mucilage drainage using phase field method.

Authors: Omid Esmaeelipoor Jahromi[1]; Ravi Patel[2]; Johan Alexander Huisman[None]; Jan Vanderborght[None]

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Rhizosphere differs from bulk soil due to the presence of root mucilage, which affects physical, chemical, and microbial processes. It is well known that the rhizosphere responds slowly to water potential changes, which buffers changes in water content and helps keep the rhizosphere wetter than bulk soil during drying. Mucilage can affect solute transport and gas diffusion by affecting the distribution of liquid and gas phases. Despite increased recognition of the importance of mucilage, there still is a lack of models that describe the connectivity between different phases in the pore space of the rhizosphere during wetting and drying. The main challenge for model development is the complex concentration-dependent behaviour of mucilage. At low concentrations, mucilage is more like a liquid, whereas at higher concentrations, dry mucilage becomes a solid. In between, a viscoelastic state is observed where mucilage can be considered as a hydrogel.
In previous work, we have developed a model based on a lattice spring method (LSM). This model was able to simulate the distribution of mucilage in the dry state at the pore scale. However, for wetter states, it is necessary to consider additional physical phenomena like surface tension, contact angle and viscoelasticity. In this study, we therefore aim to develop a Lattice-Boltzmann simulation framework to simulate two phase flow involving mucilage. To capture the interface between the two phases, a phase-field method will be used for interface tracking as this approach has gained considerable attention in recent years. The simulations will proceed as follows. We first assign the properties of a Newtonian fluid to the mixture of water and mucilage and calculate the equilibrium distribution of the liquid phase (mixture of water and mucilage) and gas in a simple pore geometry. Then, the water content will be gradually decreased, which will lead to an increase of mucilage concentration. This will in turn affect the viscosity, surface tension and contact angle, which will result in the emergence of the required viscoelastic behaviour of the mixture. For each of the water contents, the distribution of liquid (or hydrogel) and gas phases will be calculated.
The newly developed model will provide us with new perspectives on hydrodynamic processes within the pore space of the rhizosphere. In addition, the model will help to better understand processes that strongly depend on hydraulic dynamics in the rhizosphere, such as solute transport, root penetration resistance, rhizosheath formation, and microbial activity.

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Energy Transition Focused Abstracts:

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Evaluation of gypsum-rich rock formations in the context of geological carbon sequestration

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Geological carbon sequestration is a promising means of reducing atmospheric carbon dioxide emissions by capturing CO2 gas and storing it long term in subsurface porous rock. The goal of geologic carbon sequestration is to sequester CO2 in an aqueous, solid, or pure gas form so it cannot re-enter the atmosphere. In this study, a gypsum-rich rock sample from Cassville, Georgia was analyzed as a potential injection site for carbon sequestration. Before injection, it is of the utmost importance to have an accurate prediction of the geochemical processes that will occur with the addition of supercritical CO2 to the formation. The specific reactions studied include the initial acidification of the brine present in this sample and the reactions between CO2 and gypsum: dissolution and precipitation of both gypsum and calcite. These dissolution reactions are highly dynamic and the goal of the models is to provide an accurate prediction of the rate, extent, and impact of geochemical the reactions in the formation. The reactive transport modeling software Crunchflow was used to model these dynamic processes. Images of the sample were taken using a scanning electron microscope (SEM) with a backscatter electron (BSE) detector. These images were used to calculate the porosity of the sample and mineral accessibility as well as create a segmented mineral map. This data was used to inform the reactive transport model. The results of this model provide predictions of changes in this formation including porosity, permeability, mineral precipitation and dissolution. This project is supported by the Southeast Regional CO2 Utilization and Storage Partnership (SECARB-USA), funded by the U.S. Department of Energy

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MS21 / 603

Convection in Salt Lakes

Authors: Matthew Threadgold[1]; Cédric Beaume[1]; Lucas Goehring[2]; Steven Tobias[1]

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Salt lakes occur worldwide in arid environments and are spectacular geological features, displaying breathtaking patterns on their surface. In these lakes, the only outflow of fluid is due to evaporation and dissolved salts in the groundwater precipitate at the surface, leading to the growth of a salt crust. Under the right conditions, ridges can be observed in the crust, resulting in a remarkable polygonal pattern. Understanding the formation of these distinct polygonal patterns is key to monitoring the dust emission potential of salt lakes. We model salt lakes using a 3D porous medium which is subject to a uniform through-flow, parameterised by the Rayleigh number and the lake depth. This leads to a base state characterised by exponentially-distributed salinity that is unstable for large enough Rayleigh numbers and whose instability leads to buoyancy-driven convection supported by salinity plumes. We simulate the dynamics numerically and analyse the sequential stages of the instability using characteristic properties of the system (e.g. average salinity fluxes, average and dominant pattern wavenumbers). Initially, linear growth away from the base state develops and patterns emerge in the surface flux of salinity. As nonlinearity becomes important, a net transport of salinity away from the surface builds. Eventually, plumes penetrate deep into the domain and the dynamics approach a chaotic but statistically-steady end-state, characterised by patterns which are strikingly similar to those observed in situ.

Participation:

In-Person

References:

J. Lasser, J. M. Nield, M. Ernst, K. Volker, G. F. S. Wiggs, M. R. Threadgold, C. Beaume and L. Goehring 2022 Salt Polygons and Porous Media Convection, arXiv: https://arxiv.org/abs/1902.03600
M. R. Threadgold, C. Beaume, L. Goehring and S. M. Tobias 2023 (in preparation)

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Fabrication of Synthetic Porous Media with Altered Petrophysical Properties

Authors: Sahchit Chundur[1]; Shaina Kelly[1]

[1] *Columbia University*

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The study of fluid flow in geologic porous media holds an important place in the energy transition, with relevance to low carbon energy applications such as geothermal energy production, carbon capture and storage, and subsurface hydrogen storage. Understanding fundamental petrophysical properties (e.g., porosity, permeability, saturations, relative permeability) and their relationships to one another and to other properties such as thermophysical properties is vital in creating models of subsurface activity and assessing viability of clean energy applications in new locations. However, the heterogeneous nature of geologic porous media makes it difficult to study properties in isolation in order to obtain broad scale fundamental relationships between properties.
Fabrication of synthetic porous media, such as sintered glass bead packs and sintered minerals, is a potential approach for studying petrophysical properties in isolation. Choices in the fabrication process can help reduce heterogeneity and confounding variables in order to focus on the study's properties of interest. In addition, synthetic grain packs can be used for collocated imaging, such as

3D microfluidics studies with confocal microscopy. The purpose of this project is to create a thorough methodology for fabricating sintered synthetics and evaluate the effectiveness of techniques to alter petrophysical properties of synthetic media, with porosity, permeability, pore size distribution, and wettability as the primary properties of interest. Parameters of the fabrication process such as sintering temperature and time, material size, and material composition will be adjusted in order to find the optimal specifications for fabrication, and to find the relationship between fabrication parameters and resulting properties in the material such as porosity and pore size distribution. Post-fabrication alteration processes will also be investigated to ascertain their effectiveness in modifying properties like wettability and any possible interference the processes may have on experiments with the altered porous media. Creating a framework for fabrication of synthetic porous media will streamline the process for future research and provide a foundation for researchers to isolate and investigate fundamental petrophysical properties in porous media.

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Relating Thermophysical and Petrophysical Properties in Geologic Porous Media

Authors: Sahchit Chundur[1]; Shaina Kelly[1]

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As the world economy transitions to low carbon energy, alternative subsurface energy sources such as geothermal energy have come to the forefront of energy research and investment. Understanding the mechanics of heat transfer and coupled thermal-hydrological-mechanical-chemical (THMC) processes in geologic porous media is vital in modeling and assessing the geothermal potential of rock formations. As liquid flows through fractures in the subsurface in order to extract heat, it invades the pore matrix of the surrounding rock as a function of petrophysical properties such as initial fluid saturations, porosity and wettability. This invasion, often referred to as "leak-off", informs the establishment of a saturation gradient or reactive fluid front in the matrix over time. We posit that leak-off can have a significant impact on the thermophysical properties of the rock, and by extension the behavior of heat transfer between the rock and the working fluid. The introduction of a relatively cold working fluid into the pore space decreases the average temperature of the rock unit and increases its overall heat capacity, requiring more energy input from surrounding rock to increase the temperature of the saturated rock unit and reducing the heat transfer ability of the rock. At the same time, an increase in saturation enhances the thermal conductivity of the rock unit due to liquid filling pores and coating grains, providing superior pathways of heat conductance through the rock. Understanding the dynamic nature of these properties with saturation and time in a variety

of lithologies is vital in evaluating geothermal potential and output over time.
In this work, we investigate the impact of fluid invasion on thermophysical-petrophysical properties in hot dry rock (HDR) enhanced geothermal system lithologies (e.g., granites, basalts, tuffs), low permeability systems where the introduction of injected water is the dominant influence on saturation gradients formed in the system, as well as in deep sedimentary formations (e.g., shales and sandstones) such as the Gulf Coast region, where geothermal co-development opportunities with ongoing oil and gas operations are being explored. The focus of this research lies in understanding the influence of saturation and by extension lithological and petrophysical properties on thermophysical properties and heat transfer ability of formations of interest for geothermal exploitation. The selected rock cores will be analyzed with select routine and special core analysis methods (RCA and SCAL). The cores will be tested for thermal conductivity and heat capacity at different saturations using a thermal needle measurement system, with boundary controls present to preserve saturation during heating. These measurements will be used to establish the nature of the relationship between saturation and thermal properties for each rock type, as well the influence of lithology and other petrophysical properties. These relationships will be applied to evaluate the geothermal potential of different rock types, accounting for the rate of change in saturation, porosity (for reactive rocks), and thermophysical properties over time using spontaneous and forced imbibition data. The findings will be relevant for various subsurface applications involving transport properties across the critical matrix-fracture interface.

Participation:

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Poster / 606

Evaluation of phase and inter-phase fractal dimensions during two-phase primary drainage in a microfluidic cell

Authors: Nikolaos Karadimitriou[1]; Alexandros Terzis[2]; Dongwon Lee[3]; Samaneh Vahid Dastjerdi[None]; Holger Steeb[4]

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It has been four decades since Wilkinson and Willemsen 1 introduced a new, at the time, theory of percolation, the invasion-percolation theory, as they named it. The concept was based on the fact that a displacement process between two immiscible fluids is capillarity-driven, but can be applied

also in cases where the path of lowest resistance is followed. It involves the use of the fractal dimension of the bulk invading phase in the expression of the fraction of saturation of the relevant phase, as soon as this phase becomes connected, meaning is percolating.
In this work we quantify the bulk fractal dimension of the non-wetting phase during a primary drainage process, in a microfluidic cell with the box-counting method. Twelve combinations for boundary flux conditions and viscosity ratios were experimentally investigated, in terms of the evolution of the fractal dimension of the bulk invading phase, and all the corresponding interfaces between all phases involved, namely wetting, non-wetting and solid. Based on the images acquired during the displacement processes, plots related to the corresponding fractal dimensions for all entities with saturation, capillary number and viscosity ratio were produced, as soon as percolation was established for the non-wetting phase.
Our results showed that we could reproduce the Lenormand [2] diagram in terms of capillary and viscous fingering regimes in the capillary number - viscosity ratio space. We could also identify the relative significance of each fractal dimension with respect to the flow regime. Some of them could be used, either as stand-alone information or in a complementary manner, to identify the flow regime in the space defined by the capillary number and viscosity ratio. Finally, we speculated the reasons behind the change of the corresponding fractal dimensions with respect to saturation, as a morphological information of the corresponding bulk phases and their interfaces.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS13 / 607

Adsorbed Layer Transport Dominates Thin Film Evaporation in Nano Scale Confinements

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Evaporation studies focus on the identification and characterization of heat transfer and flow dynamics in the vicinity of the solid-liquid-vapor contact line. The meniscus is often characterized by the following three regions: non-evaporating adsorbed layer, thin-film, and capillary regions. The adsorbed layer, which has a thickness on the order of nanometers, is traditionally believed to be non-evaporating due to the strong intermolecular forces producing a strong disjoining pressure that suppresses evaporation. Despite this classical view, recent molecular dynamics (MD) simulations have shown that adsorbed layer plays a significant role during thin film evaporation 1. Utilizing a

new energy-based interface detection method [2], we present nonequilibrium MD simulation results of thin film evaporation of liquid argon sandwiched between two parallel platinum plates. One end of the platinum channel is heated by energy addition, while the other end is cooled at the same rate to ensure constant energy of the simulation system. Liquid argon evaporates in the heater and travels to the condenser region. As a result, the utilized MD simulation system exhibits statistically steady transport. Here we present the shapes of the evaporating menisci for 4 different channel heights varying from 2 nm, 4 nm, 8 nm, and 16 nm, at three different wall-fluid interaction parameters and under several different heating/cooling rates. Depending on the surface wettability and applied heat flux the meniscus can be in the pinned or receding regimes. The latter case creates adsorbed layers suitable for investigating its dynamics. The higher wettability cases exhibit thicker and more stable adsorbed layers, with reduced radius of curvature (ROC) and reduced evaporation rate. They are more stable and can handle higher heat fluxes. The lower wettability cases exhibit more evaporation but can easily lead to dry out. For channel sizes less than 10 nm, the adsorbed layer and evaporating thin film regions are intertwined, and evaporation from the adsorbed layer can contribute up to 80% of the total evaporating mass flowrate. Even for the largest channel case (16 nm), the adsorbed layer contributed about 10% of the total evaporating mass flowrate [3]. The talk will focus on these findings and gear towards consolidation of our findings towards a universal behavior of adsorbed layer transport in nanoscale confinements.

Participation:

In-Person

References:

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MS01 / **608**

Multi-scale and dynamic imaging of shales and mudstone: increasing understanding of sealing ability for sub-surface storage

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Mudstones and shales are commonly the primary control on the sealing efficiency for subsurface storage applications (e.g. energy, CO2, H2, waste). However, their fine-grained and heterogeneous nature makes their full characterisation highly challenging. Here we demonstrate the multi-scale and dynamic imaging approaches that can help meet these challenges and discuss limitations and future opportunities.
Microstructures can be characterised at scales from sub- nm (<1 nm) to over 1 m, using multi-scale and multi-model imaging approaches [1-3], including X-ray tomography, Focused Ion Beam Scanning Electron Microscope and Transmission electron microscopy tomography. The majority of pores in mudstones/shales range from 0.2 nm to 3μm, and we have documented 4 major types with 3 distinct size distributions [4]. Based on the REV analysis, pore sizes, types and distribution can be upscaled via three stages from sub-nm to cm-scale[5]. The permeability is pressure dependant, ranging from 1.0×10-17 to 1.0×10-22m2 [3, 5]. CO2 adsorption is 3-7 times higher than CH4 and over 10 times higher than H2 [6]. Image based modelling has demonstrated that the non-Darcy effects (e.g., slip flow and Knudsen diffusion). Adsorption/desorption and surface diffusion takes major controls over time after injection [7].
Dynamic imaging of mudstones/shale has provided the opportunity to characterise the thermo-hydro-mechanical-chemical (THMC) properties and the coupling mechanism in mudstones/shales to investigate the sealing ability under realistic reservoir conditions. These include high temperature (from less than 10 ℃ up to 1000 ℃) [8], high pressure (e.g. confining pressure, indentation, torsion, deformation and fractures; up to 65 MPa) [9], fluids (e.g. diffusion, adsorption, flowing through, multi-phase flow) [10] and complex chemistry environment (brine and drilling fluids) [11]. Based on the dynamic behaviours observation and quantification, It can be concluded that mudstone/shales with horizontally thin-layered laminations, few fractures and less reactive minerals may act as the best caprocks.
Whilst the above has led to an improved understanding of shale/mudstone microstructure under static and dynamic conditions, significant challenges still remain regarding representivity and upscaling, experimental analysis at subsurface-realistic temperatures, pressure and chemistry, accurate estimations of the long-term behaviours and the proper monitoring techniques.

Participation:

In-Person

References:

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MS18 / **609**

The effect of upscaling the reaction rate on predictive modeling

in subsurface processes

Authors: Javad Shokri[1]; Theresa Schollenberger[2]; Senyou An[3]; Bernd Flemisch[2]; Vahid Niasar[1]

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Reactive transport is a multi-scale and multi-disciplinary process used to study various environmental and subsurface applications including geothermal utilization, carbon dioxide storage, well acidizing, and contaminant remediation. Much research has been conducted to simulate reactive transport using the Eulerian approach, Lagrangian particle tracking models, and various pore-scale models. To simulate the process on larger scales, continuum models have been used due to their fewer resources demanding nature compared to other approaches.

Eulerian (continuum) models are usually expressed with a PDE describing the transport and the interconnected reaction in the form of the Advection-dispersion-reaction equation (ADRE). In cases with homogeneous reactions, which is the purpose of this study, using the reaction constant derived from the well-mixed batch reaction results in the over-prediction of the product formation in continuum models. The reactants segregation, incomplete mixing, non-Fickian transport, and the fact that ADRE is limited in considering the effect of the local fluctuations and heterogeneity of the transport and the reaction at the pore level, have been introduced as the underlying reasons for the differences.

This discrepancy has been tackled by considering a time-dependent effective rate coefficient, a smaller dispersion coefficient different from the conservative experiment, as well as non-Fickian diffusion in time or space, using an effective constant reaction rate, and considering beta distribution for the mixing ratios within the representative elementary volume (REV). Continuum models usually need more than one calibration parameter to match the experimental results which may lead to inconsistencies if the initial or boundary conditions change which undermines the generality of these models. Instead, using pore-scale models that are capable of replicating realistic variations of velocity and reaction at the pore level is of great importance. In this manner, direct numerical simulations such as Lattice Boltzmann Method (LBM) or Pore Network Modeling (PNM) are viable tools to carry out the pore-scale simulations.

The upscaled reaction rate extracted from the pore-scale simulation by volume averaging, which reflects the effect of structural heterogeneity, and preferential flow pathways, can be utilized as an input to continuum models to amplify the reliability of the Darcy-scale, and field-scale predictions. In such a way, one can include the pore-scale chemical reactions and fluctuations in the large-scale transport in subsurface heterogeneous porous structures.

This study leverages pore network modeling for pore-scale simulations due to its fast and accurate enough computation of reactive transport phenomenon, and much less computationally demanding nature compared to direct methods. The pore-scale model incorporates incomplete mixing at the pore level by the relationship between the effective reaction constant (Keff) and the Peclet number, validated by experimental results. PNM simulations were executed on a network with a size of a REV. Upscaled reaction rates were derived by performing volume averaging on the pore-scale reaction rates and were used in the continuum model to predict the experimental results. Furthermore, the capability of this upscaling method in predicting the reactive process in a 2D heterogeneous porous medium was inspected.

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MS06-A / 611

Characterisation of multiphase flow in heterogeneous rocks

Authors: Senyou An[1]; Sojwal Manoorkar[None]; Nele Wenck[2]; Steffen Berg[3]; Conxita Taberner[None]; Ronny Pini[2]; Sam Krevor[None]

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Most porous materials in nature and even from man-made are spatially heterogeneous from nanometer(molecular) scale to kilometre (field) scale. How to accurately characterise the effect of mineralogical and topological heterogeneity on hydrodynamic properties is extensively investigated, but still an open scientific question, particularly at decimeter (core) scale. Evidence from field-scale simulation and on-site observation suggest that the multi-scale mineralogical and topological heterogeneity are dominating features for accurate estimation of fluids' migration, such as during CO2 sequestration. The establishment of local equilibrium over core scales, due to capillary pressure, has a significant impact on fluid mobilisation in heterogeneous rocks. However, how to characterise the core scale heterogeneity in a complex rock (e.g., carbonate) is still not well addressed. Therefore, we sought to develop a robust algorithm to characterise the dependence of two-phase flow on the spatial distribution of topological and hydrodynamic properties using both CT-based imaging technology and the continuum-scale simulation approach. We subjected core-scale characterisation for two sandstones and three carbonate rocks, to compute the heterogeneous distributions of porosity, capillary pressure, as well as absolute permeability. Here, we concluded that the proposed algorithm is able to effectively and reasonably construct the 3D core-scale model using limited experimental information.

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Energy Transition Focused Abstracts:

612

Free energy of water confined in porous media.

Authors: Chao Zhang[None]; Lingyun Gou[None]; Shaojie Hu[None]; Ning Lu[None]

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In the mid-20th century, harnessing of thermodynamics in describing water movement in soil, viz the concept of water potential, marks the emergence of modern soil physics, unsaturated soil mechanics, and vadose zone hydrology. Yet to date, a seamless linkage between thermodynamics and water potential is still missing, leading to several long-lasting dilemmas regarding soil properties, for example, abnormal soil water density, peculiar film water viscosity and relative permittivity, pore water pressure, and water freezing temperature depression. Here, a thermodynamic framework is established by synthesizing recent advancements in soil-water interaction. The classical thermodynamic concepts are revisited, highlighting the difference between macroscopic systems commonly treated in conventional theories and the intermolecular scale system subject to external fields. Soil water is conceived as an intermolecular scale open thermodynamic system subject to external fields of gravity, osmosis, and adsorption. The formulated thermodynamic framework is verified by reducing to the conventional definition of matric potential and a recently proposed unitary definition. The accuracy of the framework is further justified in terms of mechanical equilibrium criteria. The framework predicts the existence of spatially varied pore water pressure in soil pores and can serve as the theoretical basis for reconciling the physical origin of abnormal soil behavior such as water density, film water viscosity, relative permittivity, and negative or positive pore water pressure.

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Energy Transition Focused Abstracts:

Poster / 613

Error estimates for the scalar auxiliary variable (SAV) scheme to the Cahn-Hilliard equation

Authors: Shu Ma[1]; Weifeng Qiu[1]; Xiaofeng Yang[2]

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The optimal error estimate that depending only on the polynomial degree of ε^{-1} is established for the temporal semi-discrete scheme of the Cahn-Hilliard equation, which is based on the scalar auxiliary variable (SAV) formulation. The key to our analysis is to convert the structure of the SAV time-stepping scheme back to a form compatible with the original format of the Cahn-Hilliard equation,

which makes it feasible to use spectral estimates to handle the nonlinear term. Based on the transformation of the SAV numerical scheme, the optimal error estimate for the temporal semi-discrete scheme which depends only on the low polynomial order of ε^{−1} instead of the exponential order, is derived by using mathematical induction, spectral arguments, and the superconvergence properties of some nonlinear terms. Numerical examples are provided to illustrate the discrete energy decay property and validate our theoretical convergence analysis.

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Energy Transition Focused Abstracts:

614

The Role of Iodide Ions in Wettability Alteration in Carbonates

Authors: Ahmed Gmira[1]; Dongkyu Cha[1]; Hussain Saleem[1]

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Water injection have been a successful procedure for recovering incremental crude oil from carbonate reservoirs. Recently, the concept of tuning the injected water composition, either by altering the salinity or the ionic composition have gained a significant momentum in the oil industry, encouraged by laboratory and field tests results. Both strategies can make a multiscale adjustment at the fluid-fluid and fluid-rock interfaces, in favor of oil recovery enhancement. However, salinity tuning and ionic composition tailoring have their own challenges and limitations.
In this study, we are investigating the approach of a practical concept in enhanced oil recovery with the addition of Iodide ions in a very small concentration without further treatment. Iodide ions are added to high and low ionic strength brines with different concentrations (500 ppm, 1000 ppm, 2000 ppm and 5000 ppm) to formulate an optimum injected water composition. Contact angle and interfacial tension measurements with selected crude oil are utilized to screen the effect of iodide ions concentration and to study the effect on carbonate rock wettability and crude oil-brine interface. Zeta potential and advanced Sum Frequency Generation (SFG) spectroscopy are utilized to investigate the electric charge variations and to capture the chemical structure changes at the interface.
The initial results show a limited effect of iodide ions on crude oil-brine interfacial values while they alter significantly the rock wettability to stronger water-wet. Zeta potential and SFG measurement brings new insights on understanding the chemical structures at the crude oil-brine interface and how the presence of iodide ions is affecting the interface organization and the structure of organic and inorganic components.
The proposed study is tackling the tailored water injection for EOR purposes from another angle: adding specific ions instead of adjusting the ions levels and ionic strengths. The novelty of this investigation is to bring together routine wettability alteration analysis (contact angle, interfacial tension and zeta potential) and Sum Frequency Generation technique to understand the effect of iodide ions at the fluid-fluid and fluid-rock interface and the potential in-situ changes at low scale. Such understanding is crucial to optimize the injected water chemistry at lower costs.

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Energy Transition Focused Abstracts:

615

Effect of ionic composition on carbonate and dolomite interfaces: a Direct Imaging at nanoscale by Cryo-BIB-SEM

Authors: Ahmed Gmira[1]; Dongkyu Cha[1]; Hussain Saleem[1]

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Water injection, showed encouraging results for oil recovery in carbonate reservoirs. An understanding of multiphase flow phenomena, fluids distributions inside the porous matrix and interfaces is critical to optimize the injected water formulation, leading to an oil recovery incremental.
Most of the laboratory studies reported so far, have been focused on characterization of crude oil-brine-carbonate system and wettability alteration at micro- and macroscale using classic measurements, including contact angle, Interfacial tension (IFT), Nuclear magnetic Resonance (NMR), zeta potential and coreflooding. However, those techniques depend strongly on carbonate heterogeneities, roughness and fluids distribution inside the pores. Thus, a direct visualization at pore scale is needed to identify fluids distribution in-situ, wettability state and potential alteration induced by tuning injected water composition.
Cryogenic high-resolution broad ion beam (Cryo BIB) equipped with energy dispersive spectroscopy (EDS) is utilized to study carbonate and dolomite-oil-brine interfaces at nanoscale and characterize the porosity and connectivity. High resolution EDS and image analysis allow for monitoring oil and brine distribution inside rock porosity, and to accurately quantify the length of rock-oil interfaces.
Experimental work has been conducted on carbonate and dolomite rock samples aged in crude oil and saturated with various brine compositions, covering the effect of monovalent and divalent ions and ionic strength variation. This study established an experimental protocol using cryogenic high-resolution broad ion beam (Cryo-BIB SEM) equipped with EDS. This technique allows the identification of fluids (oil and brine), distribution across the rock porous matrix and connectivity with clear visualization of the oil-brine-rock interface at nanoscale and dependency to the brine ionic composition.
Nanoscale characterization brings new insights into the oil-brine-rock interface and, combined with rock-fluid and fluid-fluid knowledge from previous studies, will lead to further optimized injected water and, ultimately, increased reservoirs oil recovery.

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Energy Transition Focused Abstracts:

616

A novel deep-learning based super-resolution method for improving the accuracy of petrophysical property prediction from Digital Rock Physics workflows

Author: Vishal Raju Ahuja[1]

Co-authors: Utkarsh Gupta [2]; Shivani R. Rapole [2]; Nishank Saxena [3]; Ronny Hofmann [3]; Ruarri J. Day-Stirrat [3]

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Digital Rock Physics leverages advances in digital image acquisition and analysis techniques to create 3D digital images of rock samples, which are used for computational modeling and simulations to predict petrophysical properties of interest. However, the accuracy of the predictions is crucially dependent on the quality of the digital images, which is currently limited by the resolution of the micro-CT scanning technology. We have developed a novel Deep Learning based Super-Resolution model called Siamese-SR 1 to digitally boost the resolution of Digital Rock images acquired from micro-CT scanning whilst retaining the texture and providing optimal de-noising. The Siamese-SR model consists of a generator which is adversarially trained with a relativistic and a Siamese discriminator utilizing Materials In Context (MINC) loss estimator. This model has been demonstrated to improve the resolution of sandstone rock mages acquired using micro-CT scanning by a factor of 2. Another key highlight of our work is that for the evaluation of the super-resolution performance, we propose to move away from image-based metrics such as Structural Similar-ity (SSIM) and Peak Signal to Noise Ratio (PSNR) because they do not correlate well with expert geological and petrophysical evaluations. Instead, we propose to subject the super-resolved images to the next step in the Digital Rock workflow to calculate a crucial petrophysical property of interest, viz. porosity and use it as a metric for evaluation of our Siamese-SR model against several other existing super-resolution methods like SRGAN [2], ESRGAN [3], EDSR [4] and SPSR [5,6]. Furthermore, we also use Local Attribution Maps to show how our proposed Siamese-SRmodel focuses optimally on edge-semantics, which is what leads to improvement in the image-based porosity prediction, the permeability prediction from Multiple Relaxation Time Lattice Boltzmann Method (MRTLBM) flow simulations as well as the prediction of other petrophysical properties of interest derived from Mercury Injection Capillary Pressure (MICP) simulations.

Participation:

Online

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Energy Transition Focused Abstracts:

MS07 / 617

A study of a non-equilibrium model with relative permeability hysteresis in two-phase water-oil system

Authors: Eduardo Abreu[1]; Paola Cunha Ferraz[2]; Wanderson Lambert[3]

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Non-equilibrium modeling is relevant in several physics of coupled processes, flow and transport of fluids situations in homogeneous and heterogeneous porous media systems, for instance, subject to phase transitions, hysteresis and chemical reactions, among many others complex systems (see, e.g. [1,3,4,5,6] and the references cited therein). To model the dynamics of these phenomena, the corresponding system of partial differential equations typically incorporates source terms. In this work, we are interested in analytical and computational modeling of situations for which we connect states in equilibrium, but we allow that the change of physical situation presents a non-equilibrium relaxation time. We discuss the 1D-2D behavior of the wave groups of solutions in non-equilibrium situations for a two-phase water-oil model with hysteresis in relative permeability in porous media [5,6], generalizing the previous 1D results in homogeneous medium 1 for 2D flows, in heterogeneous porous medium, linked to a two-phase water-oil system [2]. This nonlinear phenomena is given by a coupled set of time-dependent partial differential equations of hyperbolic-parabolic-elliptic mixed type. We also consider synthetic spatial multiscale models of permeability and porosity that resemble the geological properties which control fluid flow. The computational 2D non-equilibrium solutions are obtained based on a sequential operator splitting approach supported by the relaxation projection method introduced in 1. The main ingredients to obtain these solutions are shock, rarefactions and bifurcations [1,2]. We present 1D-2D solutions and discuss the nonlinearity interplay between wave

structure of such solutions in non-equilibrium situations and the high-contrast heterogeneity in porous medium.

Keywords: Non-equilibrium models; Two-phase flow; Porous media; Relaxation relative permeability hysteresis; Analytical-computational methods.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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Morphology and hydrodynamic properties of hydrates during dissociation in sediment

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Pore-scale formation and dissociation of hydrate under natural conditions can be qualitatively observed using μ-CT X-ray imaging. However, the quantitative criterion for the formation of hydrate is yet absent in the literature. In this paper, sediment with specific hydrate formation patterns and accurate hydrate saturation levels are numerically generated by integrating the X-ray computed tomography technique, morphological operation algorithm, and quartet structure generation set method. Utilising the topological information extracted from generated hydrate-containing sediments, we first propose a quantitative criterion to classify the microscopic occurrence types of hydrate. In this work, we visualised the 3D hydrate distribution using μ-CT imaging technology, as well as analysed the hydrate topology and its dynamic evolution through the proposed classification method and the extracted dual-network models. In addition, the variation of normalised permeability and tortuosity under different hydrate saturation are numerically analysed by adopting the lattice Boltzmann method. Results demonstrate that the bridging and pore-floating hydrate are the dominating patterns when the hydrate saturation is higher than 30%. Otherwise, the hydrate is more likely to exhibit cementing and pore-floating patterns in the sediment.

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Poster / 619

Evaluation of nanoparticle-based fluids with regard to the enhanced oil recovery (EOR) efficiency and energy cost of their synthesis

Authors: Anastasia Strekla[1]; Christina Ntente[1]; Maria Theodoropoulou[1]; Zacharoula Iatridi[2]; Georgios Bokias[2]; Christos Tsakiroglou[1]

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Two different types of polymer-coated nanoparticles (PNPs) were synthesized, stabilized in aqueous solutions of salts (NaCl, CaCl2) and used to prepare Pickering oil-in-water emulsions for enhanced oil recovery (EOR) from reservoir rocks: (1) PNPs of silica synthesized by free radical polymerization of the monomers 2-acrylamido-2-methyl-1-propanesulfonic acid (AMPSA) and dodecyl methacrylate (DMA) on the surface of acrylic-modified spherical silica nanoparticles 1; (2) PNPs of iron oxide

(IONP) synthesized by using the polyphenols extracted from plant leaves as reductants of ferric chloride hexahydrate or ferrous sulphate heptahydrate [2]. Visualization tests of the immiscible displacement of viscous paraffin oil by aqueous suspensions and emulsions were conducted in a transparent glass-etched pore network, and used to assess the performance of the various fluid systems as agents for EOR process, in terms of the oil recovery efficiency and an energy efficiency index.
The AMPSA-SiO2 PNPs were characterized by Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR) and thermogravimetric analysis (TGA). The structure of iron oxide nanoparticles was confirmed with X-ray diffraction (XRD) analysis, and scanning-electron microscope (SEM) images and energy dispersive X-ray analysis (EDX) of solid material isolated with centrifuging. The suspended nanoparticle size distribution was determined with dynamic light scattering (DLS), while the stability of the nano-colloids was confirmed by measuring the ζ-potential as a function of the ionic strength. The interfacial properties were measured by dynamic (pendant drop) and static (duNuoy) methods, whereas the wettability was quantified by measuring the oil/water contact angle on glass surfaces. With the aid of a high energy ultrasound probe, the PNP suspensions were mixed with oil (n-C10, n-C12) to prepare Pickering emulsions, the rheological properties (shear viscosity, loss and storage moduli) of which were measured on a stress rheometer, while their stability was inspected by observing the phase separation (macro-scale) and measuring the drop size distribution (micro-scale).
To assess the EOR efficiency, two-phase flow tests were conducted under constant flow rate in the following rank: (i) a drainage step, where the brine (salt solution) saturating completely the porous medium is displaced by paraffin oil; (ii) a primary imbibition step where the residual oil of the previous step is displaced by brine; (iii) secondary imbibition step, where the residual oil of the previous step is displaced by PNP-based fluid (Fig.1). The oil saturation was measured as function of time with image analysis of successive snap-shots captured by a CCD camera [3], and the transient response of the pressure drop across the porous medium was recorded with the aid of two pressure transmitters and a data acquisition card. Comparative analysis of the oil recovery efficiency and energy efficiency index, attained by all tested nano-colloid suspensions and Pickering emulsions, allowed us to classify them, and select the most efficient ones for further studies in reservoir rocks.

Acknowledgements
The research project was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the "1st Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment"(Project Number: HFRI-FM17-361, acronym: EOR-PNP).

Participation:

In-Person

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MS18 / 620

Assessing the fate of PFAS in subsurface from experimental studies and numerical simulations at soil-column scale

Authors: Anastasios Melitsiotis[1]; Nadia Bali[1]; Maria Theodoropoulou[1]; Christos Tsakiroglou[1]

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Per- and poly-fluoroalkyl substances (PFAS) are emerging contaminants of great importance, because of their spreading in subsurface, gradual bioaccumulation and toxicity. Assessing exposure risk, developing management strategies, and implementing remediation scenarios require an accurate understanding of the fate of PFAS in subsurface. In the present work, PFAS transport in saturated and unsaturated soil columns has been studied under varying initial concentration for two type of PFAS: perfluorooctanoic acid (PFOA) and perfluorodecanoic acid (PFDA). The PFAS surface tension and PFAS / n-dodecane (n-C12) interfacial tension were measured as functions of PFAS concentration and salinity with static (DuNouy ring) method, and fitted to Langmuir-Szyszkowski equation (Fig.1a,b). The capacity of PFAS solutions to emulsify non-aqueous phase liquids (NAPLs), commonly trapped in the saturated zone, was investigated by mixing PFAS solutions with n-C12 at various volume ratios with the aid of an ultrasound probe, inspecting their stability optically, and measuring transient changes of the shear viscosity. Moreover, the effects of PFAS on wetting properties were analysed by measuring the contact angles of PFAS drops surrounded by either air or n-C12 on glass surfaces (Fig.1c,d). A dried sandpack was evacuated and saturated with NaCl solution with free imbibition. Unsaturated and NAPL-polluted conditions were created by injecting air or NAPL at constant flow rate, reinjecting NaCl solution and monitoring the axial distribution of water saturation with a multiple-electrode resistivity meter 1. PFAS flow tests were then conducted, and the concentration of PFAS was measured in aqueous samples collected at the outlet port with the methylene blue active substances (MBAS) method and UV-Vis spectrophotometry [2]. The spreading of PFAS in the soil column was simulated with a 3D field scale Computational Fluid Dynamic model which simulates the PFAS transport by solving the Navier Stokes equation inside infinite domain (field scale), where convection, dispersion and adsorption (on solid interfaces and air/water interfaces) terms were included. The simulations were developed on Comsol Multiphysics platform [3] and the numerically predicted PFAS concentration breakthrough curves under saturated and unsaturated conditions were compared with corresponding datasets of PFAS flow tests in soil column.

Acknowledgements
This work was performed under Grant Agreement 101037509 —SCENARIOS —H2020-LC-GD-2020 / H2020-LC-GD-2020-3 (project title: "Strategies for health protection, pollution Control and Elimination of Next generAtion RefractIve Organic chemicals from the Soil, vadose zone and water"-acronym "SCENARIOS") supported by the European Commission.

Participation:

In-Person

References:

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MS18 / 621

4D Study of Groundwater Remediation Techniques at Pore-scale

Authors: Pavel Kazakovtsev[1]; Tannaz Pak[1]; Meezanul Islam[1]; Nathaly Lopes Archilha[2]

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Groundwater remediation is a pressing issue in the modern world. Some regions of the UK, such as Southeast England, take more than 75% of their public water supply mainly from Chalk aquifer (Groundwater resources in the UK, 2022). In Brazil, almost 37% of the cities are supplied exclusively with groundwater. Study by Lunardi et al., (2021) highlighted high susceptibility to groundwater pollution of regions, where pollutant source, such as industry, is present. The studies performed on methods similar to ones studied in this work usually do not study what is happening on pore-scale. Such study is performed by Pandey, Sharma and Saha (2022) on nZVI nanoparticle production techniques, or by Chen et al., (2021) on slow-release potassium permanganate. This highlights a knowledge gap in the modern understanding of these remediation techniques.

In this work, a dataset on nZVI nanoparticle reaction with TCE (trichloroethane) is studied. TCE is a DNAPL –Dense non-aqueous phase liquid. These compounds are challenging to be removed from groundwater reservoirs via conventional means, as they are almost immiscible in water, and are difficult to remove from the porous medium. Therefore, nanoparticles used for remediation of such reservoirs have to be able to reach the contaminant. The dataset was obtained via X-ray microtomographic scanning (X-ray micro-CT) and allows for 4D (3D + time) study of the processes, happening on the pore-scale. The dataset was captured at Diamond Light source by Dr. Tannaz Pak. This study is performed via specialised software, such as Fiji (ImageJ), Avizo and MatLab.

In addition to this, a new setup has been developed for column experiments. This setup gave us the possibility to investigate liquid and particle dynamics on a larger scale, across a column of approximately 36 cm long 3.5 cm in diameter. With this setup we were able to measure particle distribution through the column after several nZVI injections on different porosities. Particle distribution was assessed via magnetic susceptibility sensor. Each material loaded into the column is initially characterised by a breakthrough curve, evaluated via conductivity of NaCl brine. Subsequent breakthrough curves for nanoparticle injections are evaluated via magnetic susceptibility sensor. The experimental data of the breakthrough curves is then analysed with MnMs, to confirm the results of the experiment and get a better insight into nanoparticle mobility.

In addition to that, the experiment on porosity influence on the efficiency of nanoparticle remediation was performed. This experiment involved saturating porous medium with nitrate-contaminated water and injecting nanoparticle suspension into the column. Parallel to the column experiment, a reference batch test was performed, with the same concentrations of nitrates and nZVI, but in absence of any porous medium. The results of this experiment were then compared with each other, to assess the influence of presence of porous medium and porosity on decontamination efficiency.

Participation:

In-Person

References:

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622

A poroelasticity theory for soil incorporating adsorption and capillarity

Authors: Chao Zhang[1]; Shaojie Hu[1]; Zemin Qiu[None]; Ning Lu[2]

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Adsorption and capillarity, in the order of high free energy to low, are the two soil–water interaction mechanisms controlling the hydro-mechanical behaviour of soils. Yet most of the poroelasticity theories of soil are based on capillarity only, leading to misrepresentations of hydro-mechanical behaviour in the low free energy regime beyond vaporisation. This inability is reasoned to be caused by two major limitations in the existing theories: missing interparticle attraction energy and incomplete definition of adsorptioninduced pore-water pressure. A poroelasticity theory is formulated to incorporate the two soil–water interaction mechanisms, and the transition between them –that is, condensation/vaporisation, by expanding the classical three-phase mixture system to a four-phase mixture system with adsorptive water as an additional phase. An interparticle attractive stress is identified as one of the key sources for deformation and strength of soils induced by adsorption and is implemented in the poroelasticity theory. A recent breakthrough concept of soil sorptive potential is utilised to establish the physical link between adsorption-induced pore-water pressure and matric suction. The proposed poroelasticity theory can be reduced to several previous theories when interparticle attractive stress is ignored. The new theory is used to derive the effective stress equation for variably saturated soil by identifying energy-conjugated pairs. The derived effective stress equation leads to Zhang and Lu's unified effective stress equation, and can be reduced to Bishop's effective stress equation when only the capillary mechanism is considered and to Te rz ag h i's effective stress equation when a saturated condition is imposed. The derived effective stress equation is experimentally validated for a variety of soil in the full matric suction range, substantiating the validity and accuracy of the poroelasticity theory for soil under variably saturated conditions.

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Energy Transition Focused Abstracts:

Poster / 623

Effects of time-dependent velocity fields on the dynamics of chemical transport in porous media

Authors: Dan Elhanati[1]; Ishai Dror[1]; Brian Berkowitz[1]

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The dynamics of a migrating chemical plume in a porous medium can be affected by different chemical processes (e.g., sorption, retention, precipitation and dissolution, complexation, reaction), as well as by the physical properties of the medium and flow field (heterogeneity of the medium, porosity and permeability, fluid velocity). Groundwater input in natural systems can vary over a wide range of time scales, due to different natural phenomena (e.g., day and night cycles, season variability, long term climate changes) and anthropogenic activities (e.g., groundwater extraction and injection, irrigation, construction). These variations in input give rise to a time-dependent (TD) velocity field, which in turn may influence the dynamics, mixing, and reaction rates of a migrating chemical plume. Anomalous transport, which is ubiquitous in many groundwater systems and has been shown to yield longer than expected (non-Fickian) tails of migrating chemical plumes, is of particular interest in this context. In this study, macroscopically 1D transport of a conservative chemical species through sand columns was quantified by tracer measurement at the column outlet. Transport in these columns is known to display distinct, non-Fickian tailing of the breakthrough curves. Different TD velocity field conditions were compared to study how the transient water input affects the resulting tracer breakthrough curves. A stochastic-based numerical model was employed to interpret the results. The analysis shows that different TD conditions, which retain the average discharge of a comparable constant-velocity system, yield similar, long-tailed breakthrough curves to those of the constant-velocity case. These breakthrough curves can be interpreted in terms of the continuous time random walk (CTRW) framework. We then analyze the sensitivity of the CTRW to the occurrence of abrupt velocity changes, by addressing the choice of particle transition times and distances at the moment of velocity change, and show that the CTRW matches the experimental results obtained in the column experiments.

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MS10 / **624**

Evidence of self-sealing in wellbore cement under geologic CO2 storage conditions by micro-CT, SEM and Raman observations

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In this study, reaction experiments between CO2-saturated brine and wellbore cement samples cured under different pressures were conducted to study microstructural and mineral composition changes using microcomputed tomography (micro-CT), scanning electron microscopy (SEM) and Raman spectroscopy. The CT images of post-CO2 exposure cement samples showed a dissolution-precipitation-dissolution pattern at the exterior of the samples. The dissolution in the inner hole of the samples, however, was not significant. Instead, only CaCO3 precipitation was observed in the inner hole. CaCO3 precipitation in the inner hole contributes to selfsealing of the cement, which reduces the risk of CO2 leakage through wellbore cement. According to CT and SEM observations, a higher curing pressure caused more precipitation of CaCO3, which favored cement selfsealing when exposed to CO2. The appearance of a C—O peak and the disappearance of a –OH peak after reaction with CO2 were observed by Raman spectroscopy, which was attributed to cement carbonation that converted Ca(OH)2 into CaCO3. This study provides solid evidence of cement self-sealing due to cement carbonation under geologic CO2 storage circumstances.

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MS07 / **625**

Compositional Multiphase Flow Simulation: Challenges and Treatment by Deep Learning

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In recent years, we have seen increasing attention paid to multiphase flow in subsurface porous media due to issues related with enhanced oil recovery, geothermal technology, unconventional oil/gas reservoirs, geological carbon sequestration, and subsurface storage of hydrogen. One key effort prior to constructing the mathematical model governing the compositional multiphase flow is to determine the phase compositions of the fluid mixture, and then to calculate other related physical properties. For systems involving a large number of species, phase behavior calculation typically consumes majority of the CUP time in the compositional multiphase flow simulation. In this presentation, we discuss challenges in compositional multiphase flow modeling and simulation, focusing on the challenges from nonlinearity of the system, such as the nonlinearity from relative permeabilities, capillarity, and phase behaviors. As a recent effort to treat the nonlinearity from phase behaviors, we will show how machine learning can help to achieve more robust and faster prediction of phase behaviors by using supervised learning with deep neural networks. We first provide general phase splitting statements and classical flash calculation procedures using successive substitution and Newton's method. We then review our work on the fully robust and ODE-based iterative schemes for NVT flash problems and our work on its speedup using the sparse grids method. Afterwards, we present our study on a series of deep learning methods as applied to phase splitting problems. Factors in the deep learning models are investigated to understand their effect on the final result. It is demonstrated that results from the optimized deep learning model provides a robust and efficient approach for phase equilibrium calculation; if trained by experimental data, the trained neural network is more accurate than Peng-Robinson EOS-based models. Finally, we present our work in TINN (Thermodynamics-Informed Neural Network) and self-adaptive neural network for phase equilibrium calculation in conventional reservoirs as well as in unconventional reservoirs.

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MS07 / **626**

Sub-grid Modeling in a Particle-based Approach: Regularization of Non-linear Hyperbolic Conservation Law

Authors: Ranit Monga[1]; Daniel Meyer[2]; Patrick Jenny[None]

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Conventional numerical modeling techniques, with finitely resolved length and time scales, need specific treatments to include the effects of unresolved physics and solution discontinuities. In this regard, their applications to multi-scale problems involving transport in fractured media are no different. Lagrangian particle-tracking methods provide a compelling alternative to the Eulerian methods as they provide a natural connection across a multitude of scales. Further, in the context of purely advective transport, the absence of numerical diffusion makes them better placed to capture solution discontinuities, if any.

In this work, we present a stochastic particle-based framework which models reactive multiphase transport in porous media characterized by highly conductive fractures and a permeable matrix. Thereby, we use an Embedded Discrete Fracture Model (EDFM) where large fractures are resolved with lower dimensional representations [Deb and Jenny, (2017)] Macroscopic transported quantities, e.g., phase-saturation, are modeled in the essence of particle ensemble statistics.

We present a flux-conservative stochastic particle-tracking scheme tailored to EDFMs, and we illustrated its applicability for advective solute transport. Therein, we devised the probability of inter-continuum particle transfer which is particle trajectory-specific. Further, we extended this scheme to model saturation evolution in two-phase flows. Solutions of the opted non-linear hyperbolic transport problems involve discontinuities. Hence, we added minimal diffusion to the system, and to this end, an adaptive diffusion coefficient is proposed. It is inspired by the Smagorinsky-model [Smagorinsky (1963); Lilly (1966)] developed in the context of Large Eddy Simulations of turbulent flows, and it is active only in the vicinity of a saturation fronts, and thus is not overly diffusive.

The new particle-tracking scheme correctly captures the sharp saturation profiles of 1-D Buckley-Leverett problems. It is shown how the adaptive diffusion coefficient can be generalized for a wide range of flow scenarios including those with buoyancy. As a part of this exercise, comparisons of 2-D particle-based solutions are compared with those from a suitable Eulerian approach. Eventually, the capability of the overall framework for a large-scale fracture model is assessed. Subsequent research includes modeling of sub-grid processes, e.g., dissolution of one phase into the other [Tyagi (2011)] and liquid phase-solid matrix interactions. This warrants, once again, a probabilistic approach to model the transitions of particles in the state space.

Participation:

In-Person

References:

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Low cost 3D printing of electrically conductive porous media for gas diffusion layers

Authors: Yann Dumay[1]; Volker Schulz[1]; Eric A. Chadwick[2]

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The functionality of many electrochemical devices such as fuel cells, electrolysers or batteries rely on an electrically conductive porous media. Specifically, in Polymer Electrolyte Membrane (PEM) fuel cells, the gas diffusion layer (GDL) is used to distribute the gases, conduct the electrons and transport the generated water from the reaction sites to the flow fields in the bipolar plates 1. Due to these requirements, the most common material for GDLs is a carbon paper which is partially covered with polytetrafluoroethylene [2]. Mathematically, carbon paper is a heterogeneous media composed of randomly distributed carbon fibres, defined by its average transport properties, such as porosity, permeability, and conductivity. These properties strongly depend on the manufacturing process and can differ significantly throughout the media . Using carbon paper as GDL material, it is difficult to the optimize the PEM fuel cell over a wide range of operation conditions, i.e. output power and relative humidity of the gases. Numerical simulations show that tailored porous media, i.e. with locally different properties, can improve fuel cell performance [3,4]. However, due to the trade-offs between performance, manufacturability, and cost, designing a commercial GDL is a highly challenging task.

Here, we present an approach to generate electrically conductive porous media based on additive manufacturing with a low cost Fused Deposition Modeling (FDM) printer. FDM is an additive manufacturing method consisting of the extrusion of material trough a nozzle, which is deposited in successive layers to create a 3D object. Usually, the materials used with FDM printers are polymers-based filaments. The polymer is chosen according to the requirements of the printed part, e.g. Acrylonitrile Butadiene Styrene is used due to its relatively high melting point, or Polylactid (PLA) as a low-cost bioplastic. Moreover, some filaments available on the market are composite materials, which can improve the mechanical properties of a printing part or are electrically conductive. Therefore, using FDM to design and optimize GDL is very accessible due to the simplicity and speed of the process in addition to the low cost of the material.
In this study, we used an electrically conductive PLA from Protopasta (Vancouver, Canada), and a standard FDM printer (Ultimaker 2+). The aim of this study was to print thin, porous media with heights up to 150 microns and pore diameters of about 100 microns. This was challenging since the diameter of the nozzle head is about 250 microns. Nevertheless, in this study we have shown that it is possible to print structures with sizes down to 100 microns by using specific infill pattern parameters,. Moreover, the infill pattern can be modified to obtain either regular patterns (left figure), or random heterogeneous structures (right figure). The electrical conductivity of these 3D printed porous media is highly dependant on its structure. We measured values between 0.6 and 0.8 [5]. In conclusion, the 3D printed parts from the electrically conductive PLA can be used for the rapid prototyping of novel GDL structures.

Participation:

In-Person

References:

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Poster / 630

Modeling and simulation of reactive two mineral systems

Authors: Stephan Gärttner[None]; Peter Frolkovic[None]; Peter Knabner[None]; Nadja Ray[None]

Corresponding Authors: nadja.ray@ku.de, peter.frolkovic@gmail.com, knabner@math.fau.de, stephan.gaerttner@fau.de

We set up a pore-scale model for reactive flow and transport in an evolving porous medium. We take into account dissolution/precipitation reactions of two competing minerals. The resulting space and time-dependent structural dynamics are included into the model by means of a level-set formulation.

We derive the corresponding effective model by formal two-scale asymptotic expansion. This includes dynamically changing time- and space-dependent ‘effective’ hydrodynamic parameters such as porosity, reactive surface, diffusion, and permeability.

We present numerical simulations with application to dissolution of calcite and dolomite of the pore-scale as well as of the effective model.

Participation:

In-Person

References:

Gärttner S., Frolkovič P., Knabner P., Ray N.:
Efficiency of micro-macro models for reactive two-mineral systems
Multiscale Modeling & Simulation 20
2022

DOI: 10.1137/20M1380648

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Energy Transition Focused Abstracts:

MS12 / 631

Scaled Physical Modeling of CO2 Cyclic Injection Process in A Heterogeneous Unconsolidated Sandstone Formation using Additive Manufacturing and Geotechnical Centrifuge Technologies

Author: Daniel Cartagena-Pérez[1]

Co-authors: Alireza Rangriz-Shokri [1]; Gonzalo Zambrano [1]; Richard Chalaturnyk [1]

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To integrate the complex interplay of mechanics of gaseous solvent injection, reservoir deformation, and near-wellbore formation collapse, we designed and manufactured a highly-instrumented scaled laboratory experiment, capable of simulating and monitoring the cyclic CO2 injection process in heavy oil reservoirs at in-situ conditions. In this work, we present the application of a 2-meter beam geotechnical centrifuge for scaled physical modeling of multiphase flow (i.e. live heavy oil) in a 3D printed rock specimen under different triaxial stress states.

The new centrifuge cell consists of a vertical loading system to emulate overburden, an 8-arm horizontal loading system to induce stress anisotropy, and a production unit to collect the produced fluids and the collapsed sand grains. Heterogeneity was included in the 3D printed porous rock in the form of high permeability channels near the perforations of a scaled wellbore within the physical model. The sample was first saturated with water, followed by dead oil and live oil. The 500 kg setup was spun at 30 times the gravitational acceleration (approximately 120 revolutions per minute) before opening the wellbore and initiating the fluid production.

Upon the completion of the test, the 3D printed sample was taken for physical inspection. Changes in initial fluid saturation and the rock structure were observed around wellbore and high-permeability channels due to the stress concentration. The findings highlight the key role of coupled flow and geomechanics processes in understanding of the porous media. Moreover, the new experimental tool enables one to study the multi-phase flow in deformed porous media at different scales and more representative in-situ stress boundary conditions.

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MS07 / **633**

A Lagrange multiplier method for the fully dynamic Navier-Stokes - Biot system

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We develop a mixed finite element computational model for the interaction between a free fluid and a poroelastic medium . The free fluid flow is governed by the time-dependent incompressible Navier-Stokes equations, while the poroelastic region is governed by the Biot system. A Lagrange multiplier method is employed to impose weakly the continuity of flux. Under a small data condition, existence, uniqueness, and stability of the semi-discrete continuous-in-time and fully discrete formulations are proved. We further establish error estimates for the fully discrete method. A series of numerical experiments are presented to verify the theoretical convergence rates and illustrate the applicability of the method to modeling arterial blood flows.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS19 / **634**

Electro-diffusion through montmorillonite gels

Author: Fatiha Bouchelaghem[1]

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Numerous experimental and theoretical studies, conducted from the atomic to the field scales, have demonstrated that macroscopic properties of smectite clays, such as ion diffusivity and swelling

potential, are governed by the underlying hierarchical organization of pores, and by the morphology and permanent charge deficit of the montmorillonite layers that form its finest fraction.

Besides, as observed by (Hetzel et al, 1994; Keller et al, 2014; Nakashima, 2003; Pusch, 2001), bentonite hydration is associated with delamination and exfoliation of a fraction of the montmorillonite layers, resulting in the development of a network of colloidal clay gels of low density within the mesopores. However, very few data are available concerning ion diffusivities in montmorillonite gels (Nakashima, 2003), the matter being complicated by electrostatic interactions that develop at the interface between the elongated layers and the electrolyte solution.

In this context, real microstructures have been employed to investigate ion transport by diffusion through montmorillonite gels and water-saturated bentonite.
Using image analysis, Transmission Electron Micrographs (TEM) of hydrated montmorillonite layers (Fu et al, 2011; Hetzel et al, 1994; Tester et al, 2016; Whittaker et al, 2020) have been processed in order to extract the contours of the layers, and to determine microstructural parameters such as local orientations and bending radii. The same image analysis procedure is then employed on digitized TEM of water-saturated bentonite (Pusch, 2001) in order to obtain the contours of the different phases: non-smectite grains and other components impervious to ion diffusion, clay gels of varying density, and mesopores.

The modeling approach followed is the Homogenization of Periodic Media. At the scale of hydrated montmorillonite layers, diffusion of ionic solutes is modeled by considering chemical and electrostatic interactions in the vicinity of the clay platelets'surface (using Nernst-Planck equation, Poisson's equation of electrostatics and appropriate boundary conditions for each ionic species transported and for the electric potential). By writing the system of equations in dimensionless form, two classes of problems arise (one strongly coupled and nonlinear, one weakly coupled and linear) depending on the respective orders of magnitude of the electrolyte concentrations and the surface charge density.

Following the hierarchical description of bentonite microstructure depicted above, homogenization computations are performed first on montmorillonite gels, and the effective properties computed at the mesoscopic scale are then used to identify the diffusion behavior at the bentonite scale.

Ion distribution and electric potential maps are obtained by solving the local problems within the interlayer space, displaying cation inclusion and anion exclusion effects (Figure 1).
The mesoscopic transport equation is derived through upscaling, and leads to the identification of the effective diffusion tensor and effective coefficients expressing the coupling between the electric potential and ion concentration gradients. The diffusion tensor anisotropy is confronted with the microstructural parameters measured on the digitized micrographs.
Comparisons are made with existing models (Scheiner et al, 2013) and diffusion data obtained for low-density montmorillonite gels (Nakashima, 2003).

Finally, effective diffusivities identified for Montmorillonite gels are used to compute the macroscopic diffusion tensor for Wyoming bentonite microstructures as in (Bouchelaghem,2018).

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 635

Hallmarks of chaotic mixing in two dimensional unsteady porous media flow

Authors: Kevin Pierce[None]; Gaute Linga[1]; Marcel Moura[2]

[1] *University of Oslo*

[2] *PoreLab - University of Oslo*

Corresponding Authors: marcel.moura@fys.uio.no, gaute.linga@mn.uio.no, kevin.pierce@mn.uio.no

Solute mixing in steady porous media flows is easy in three dimensions. Flows elongate solute filaments exponentially fast, and this "chaotic" elongation enables molecular diffusion to rapidly produce uniformity. In two dimensional steady flows, filament elongation is much slower, meaning mixing can be far less efficient. However, many porous media such as biological tissues and geological fractures can have a two-dimensional character, leading us to question if these media can also support chaotic mixing. In this talk, we share experimental evidence that two dimensional porous media flows can exhibit chaotic mixing whenever the underlying flow is made unsteady, for example by introducing (1) a second fluid phase or (2) transverse flow oscillations. In the oscillating flow case, we further demonstrate that the mixing efficiency has resonances as the amplitude and frequency of oscillations varies. These results constitute the first experimental evidence for chaotic mixing in two dimensional systems, and they lend new understanding from which we might one day produce efficient geologically inspired mixers.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS17 / 636

A novel local-minima 3D image segmentation method for fluid flow in low-resolution porous material images

Authors: Rui Li[1]; Yi Yang[1]; Wenbo Zhan[1]; Jianhui Yang[2]; Yingfang Zhou[1]

[1] *University of Aberdeen*

[2] *Geoscience Research Centre, Total E&P UK Limited, UK*

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Image segmentation is a prominent process in Digital Rock Physics analysis. It directly affects the accuracy of the fluid-flow simulation in porous mediums. The accuracy of conventional global thresholding segmentation depends on image resolution. Coarse-resolution digital rock images are normally used to avoid high computation costs in processing high-resolution images that usually have more accurate results. But the image segmentation implemented on the low-resolution images becomes more arbitrary and thus generates less satisfying simulation results. This work develops a novel local-minima 3D image segmentation method that can improve the accuracy of simulations of fluid flow in low-resolution rock images. It adopts two global threshold values to capture the convinced pure pore and solid phase. Voxels having greyscale values between the two thresholds are assigned to a temporarily uncertain phase. A search algorithm is then applied to find the local minima in the uncertain region. These local minima are pores while the rest are solids. Indiana Limestone and Bentheimer Sandstone digital rock images scanned at different resolutions are studied to validate the local-minima segmentation method. We apply the conventional global thresholding and the proposed method to these digital models and study the pore- and throat-size distributions by extracting pore networks by a maximal-ball algorithm. The result shows that the local-minima method yields networks that are more accurate than those generated by the global thresholding method. In addition, we calculate the permeabilities of these models by a Lattice-Boltzmann method. The local-minima segmentation method yields an average absolute permeability error of 23% for the Indiana Limestone and 13% for the Bentheimer Sandstone, whereas the global thresholding method yields 202% and 83.67% errors, respectively. The result demonstrates that the carbonate rock is impacted more by the coarsening of image resolutions. Our segmentation technique can improve the overall accuracy of fluid flow simulations in low-resolution digital images.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS08 / **637**

Intermittent shifting of preferential flow paths in bioclogged porous media enhances mixing-driven reactions

Author: Veronica Morales[1]

Co-author: Jiahui Zhou [1]

[1] *University of California, Davis*

Corresponding Authors: zjhzhou@ucdavis.edu, vermorales@ucdavis.edu

Microorganisms can establish organized biofilms in many natural and engineered porous media systems with significant advantages to applications such as biofilm barriers to groundwater pollution. The formation of thick biofilms can change the pore structure and consequently alter the hydrodynamics and reactive transport in porous media. Yet, the impact of preferential flow path formation and spatiotemporal rearrangement on overall system reactivity in bioclogged systems remains poorly understood. A two-dimensional pore-scale numerical model was developed to examine the effect of mixing and reaction efficiency upon biofilm development, biomass growth scheme, and preferential flow path stability. Simulations of water flow and solute transport in the porous medium were coupled to a biomass growth and attachment model scheme for a period of 400 hours. Four biomass growth models were tested, including i) no decay, ii) kinetic decay, iii) degradation, and iv) mechanical detachment. Our results indicate that i) permeability reduction and variations in the biomass fraction reached a similar and quasi-constant value after 100 hours for all growth models, ii) the shifting location of preferential flow paths only occurred when biomass growth was overcome by the combination of shear forces with biomass decay and/or degradation, iii) flow stagnation zones enhance the formation of strong concentration gradients, and iv) the preservation of high overall reactivity within the system requires intermittent shifting in the location of preferential flow paths.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

638

Understanding the influence of biomineralization kinetics on pore morphology by evaluating geometric characteristics: Internal specific surface area, tortuosity, and pore-size distribution

Author: Daehyun Kim[1]

Co-authors: Hojeong Kang [2]; Jiwon Choi [2]; Tae Sup Yun [2]; Toshiro Hata [3]

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In this study, evolving complexity of pore morphology during the biomineralization process was evaluated with the selected geometric parameters, the internal specific surface area, tortuosity, and pore-size distribution. Biomineralization involving ureolytic microorganisms that promotes calcium

carbonate mineral precipitation has been widely investigated for various engineering applications since it can enhance the strength or reduce the permeability of soils. Previous studies have commonly tried to establish the empirical correlations between the precipitated mineral contents and modified engineering properties of treated soils, mostly Unconfined Compressive Strength (UCS) and permeability. However, the modified engineering properties of treated soils are affected by not only the precipitated mineral content but also pore morphological change due to the treatment. Even at an equal precipitation level, the pore morphology can be varied based on the precipitation patterns and its locality which might be highly affected by the precipitation kinetics.
The selected geometric parameters in this study, the internal specific surface area, tortuosity, and pore-size distribution represent pore morphology which can significantly affect both the reactive transportation phenomena of fluid in porous media and the development of force chains in the soil system. To investigate the impact of the biomineralization kinetics on the alteration of pore morphology, three biomineralization cases with different reaction rates (fast-, intermediate-, and slow-reactions) were assumed and computationally simulated in a 2D porous medium which was obtained from a cross-sectional view of the 3D X-ray CT scanned sandy specimen. The tortuosity and internal specific surface area were measured at every 1% increase in mineral content. The findings highlight that the tortuosity exponentially increased as precipitation proceeded after certain levels of precipitation while the porosity linearly dropped. The normalized internal specific surface area showed distinguished trends, increasing (in fast-), maintaining (in intermediate-), and decreasing (in slow-reaction). The increased complexities of pore structure based on the predominant precipitation sizes were well presented in the pore size distribution curves.

Participation:

Online

References:

Kim, D., Mahabadi, N., Jang, J., & van Paassen, L. A. (2020). Assessing the kinetics and pore-scale characteristics of biological calcium carbonate precipitation in porous media using a microfluidic chip experiment. Water Resources Research, 56(2), e2019WR025420.

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Energy Transition Focused Abstracts:

MS14 / 640

Improved techniques for uncertainty quantification of foam flow in porous media

Authors: Luisa Silva Ribeiro[None]; Berilo de Oliveira Santos[None]; Gabriel Brandão de Miranda[None]; Grigori Chapiro[1]; Bernardo Rocha[1]; RODRIGO Weber dos SANTOS[2]

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Computational models can predict and improve our understanding of multiphase flow in porous media. In this field, the task of uncertainty quantification is of paramount importance when developing and evaluating mathematical models aimed at the design and prediction of complex processes

such as enhanced oil recovery techniques. One promising Enhanced-Oil-Recovery technique is the injection of foam in the porous medium, since foam injection reduces gas mobility and increases apparent viscosity, thus improving reservoir sweeping and increasing recovery efficiency. This work focuses on parameter estimation and uncertainty quantification of the foam flow in porous media. In particular, we present an uncertainty quantification approach based on surrogate models and Bayesian inference to evaluate how these techniques can reduce uncertainties and improve physical understanding and parameter estimation of foam flow in porous media. Our results suggest that the new framework based on Bayesian inference and surrogate models enhances parameter estimation and improves the uncertainty quantification of the foam flow in porous media.

Acknowledgements. The current work was conducted in association with the R&D project ANP n 20715-9, "Modelagem matemática e computacional de injeção de espuma usada em recuperação avançada de petróleo"(UFJF/ Shell Brasil/ANP). Shell Brazil funds it in accordance with ANP's R&D regulations under the Research, Development, and Innovation Investment Commitment. This project is carried out in partnership with Petrobras.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS03 / 641

Multiscale modelling of CO2 storage in coal seams: an image-based modelling method

Authors: Yu Jing[1]; Arash Rabbani[2]; Peyman Mostaghimi[None]; Ryan Armstrong[None]

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[2] *The University of Leeds*

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CO2 geo-sequestration is a practical approach to achieve net-zero carbon target. Coal has become an optimal geological storage option due to its large adsorptive capability for CO2. However, one of the main challenges for successful CO2 geo-sequestration is the reduced injectivity that are caused by adsorption-induced swelling of coal matrix. In addition, its complex and heterogenous internal pore and fracture structure make the processes of gases adsorbing, desorbing, and transporting more

complicated compared with conventional rocks. This work aims to gain insights about the gas transport behaviours in coal by developing a coupled model to simulate gas flow multiphysics as well as dynamic coal deformation.

This work develops an image-based 3D fracture network model, called Fracture Box Model (FBNM), which is directly derived from 3D images of real coal samples. In this model, each fracture is described by arrays of box elements such that the regional change of fracture opening widths can be preserved. FBNM is used to simulate viscous flow in fractures, gas diffusion in matrix micropores, gas exchange on coal surface, coal matrix deformation (due to sorption and thermal expansion). Compared with other fracture models (e.g. discrete fracture network), FBNM can simulate such complicated multiphysical gas transport more efficiently, but also be able to simulate corresponding coal matrix deformation. By comparing permeability results between direct simulation method with FBNM, it is found that FBNM can effectively estimate the permeability of original fracture networks, but requiring significantly less computational cost. To study the implications of gas types, effective stress, gas adsorption, and thermal expansion on coal permeability, gas injection pressures, gas types, coal seam temperatures are varied and investigated in the simulations.

The FBNM developed in this work is more preferable for complicated flow transport simulations where direct simulation methods are still challenging. It provides a promising framework which could be further developed for multiphase and multicomponent flow simulations for CO2 geo-sequestration projects.

Participation:

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Energy Transition Focused Abstracts:

MS13 / 642

Investigation of Catalyst Layer and Microporous Layer Liquid Water Saturation Level in Polymer Electrolyte Fuel Cell by Operando Small&Wide Angle X-ray Scattering

Author: Kinanti Aliyah[1]

Co-authors: Anne Berger [2]; Timon Lazaridis [2]; Christian Appel [1]; Andreas Menzel [1]; Hubert Gasteiger [2]; Felix Buechi [1]; Lorenz Gubler [1]; Jens Eller [1]

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In recent years, substantial research and development endeavors are dedicated to enhancing the performance of polymer electrolyte fuel cells (PEFC) as a promising candidate for transport application. However, the power density still needs improvement for large-scale operations with one of the core

issues being water management. The convoluted water balance in the PEFC requires proper water management to ensure high cell performance. Excess water retention in the pores results in blockage of the gas diffusion to the active sites of the electrochemical reaction, thus reducing performance and efficiency. Appropriate membrane humidification is needed for high proton conductivity. The deployment of a microporous layer (MPL) located between the gas diffusion layer (GDL) and the catalyst layer (CL) has been demonstrated to enhance water management. Operando scanning small and wide angle X-ray scattering (SAXS&WAXS) is utilized in this study as a practicable tool to explore the water level in the nanoscale CL and correlate it with the neighboring MPL material design at the cSAXS beamline of the Swiss Light Source. The use of a small beam size (≈7x30 microns) and ≈0.6 microns vertical step size resolves the bulk CL (≈7 microns thick) and additionally allows for a precise registration in case of membrane movement during operation. Due to the electron density difference between solid-void and solid-liquid interfaces, the water saturation level is quantifiable (see Fig. 1a). Relevant PEFC operating conditions (80^{0}C, relative humidity 100%, 1.7 and 3 bar abs.) were enforced to compare the impact of two different MPL modifications (pore former inclusion, and higher PTFE content) to the water saturation of a base case MPL (Li100, 20% PTFE). The presentation will detail the material modification consequences on the CL and MPL saturation levels to reveal pore size-specific filling mechanisms. (see Fig. 1b-c).

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MS09 / 643

Finding the Representative Elementary Volume with Hill-Mandel condition

Author: Sijmen Zwarts[1]

Co-author: Martin Lesueur [1]

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The foundation of homogenisation methods rests on the postulate of Hill-Mandel, describing energy consistency throughout the transition of scales. The consideration of this principle is therefore crucial in our discipline of Digital Rock Physics which focuses on the upscaling of rock properties. For this reason, numerous studies have developed numerical schemes for porous media to enforce the Hill-Mandel condition to be respected. The most common method is to impose specific boundary conditions, such as periodic ones. However, the recent study of Thovert and Mourzenko (2020) has shown that most boundary conditions still result in the same intrinsic effective physical property if the averaging is applied outside the range of the boundary layer. From this discovery, it becomes logical to question the status of Hill-Mandel condition in porous media when homogenising away from

the boundary. In this contribution, we simulated Stokes flow through random packings of spheres and a range of rock microstructures. For each, we plotted the evolution of the ratio micro- vs macro-scale of the energy of the fluid transport outside the boundary layer, for increasing subsample size of our porous media. Here, we prove that we naturally recover energy consistency across scales when reaching the size of the Representative Elementary Volume (REV), which is a known condition for rigorous upscaling. Furthermore, we show that this ratio for the energy consistency is a more accurate indicator of REV convergence since the mean value is already known to be unitary, which adds to the initial advantage of not having to impose any specific boundary conditions.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-A / 644

An Experimental Study of Drying in Porous Media Using Novel 2D Micromodels with Dual Porosity

Authors: Md Ahsan Habib[1]; Diego Armstrong[1]; Bo Guo[2]; Yaofa Li[1]

[1] *Montana State University*

[2] *University of Arizona*

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Drying of porous media is central to a broad range of natural and engineering applications, such as soil drying, food and pharmaceutical industries and CO_2 sequestration. It is essentially a multiphase flow process, where the liquid phase evaporates and is displaced/replaced by the gaseous phases, as vapor diffuses out of the porous structure. Drying of porous media plays a crucial role in various flow and transport processes. For instance, in soil, drying and rewetting processes control water and solute and nutrient transport. In CO_2 sequestration, drying controls salt precipitation. To make drying of porous media more complicated yet more interesting, many porous solid matrices display multi-scale variability in pore structure and physical properties such as porosity and permeability. For instance, in critical zone, soil is often viewed as a hierarchical organization: primary particles of a few micrometers in size form microaggregates of hundreds of micrometers in size, which in turn form macroaggregates, effectively leading to dual porosity in the porous media. The resultant multi-scale flow dynamics and inter-/intra-aggregate interaction in this system are recognized to control numerous processes, such as water and gaseous transport. However, the underlying physics including fluid mechanics and thermodynamics, is not well understood.

To that end, the multi-phase flow of air and water was investigated using a novel 2D dual-porosity microfluidic device, with a focus on the multi-scale interaction and the role of corner film flows.

The microfluidic device, constructed in a glass-silicon-glass architecture, offers precise structure and excellent optical access. To perform the experiment, the dual-porosity micromodel was pre-saturated with DI water, which was subsequently displaced by air at a constant flow rate until a steady phase configuration was achieved typically within a few minutes. Air was then continuously injected at a constant flow rate until water completely dries out, which typically takes serval hours. The entire process was quantified using a dual-magnification micro-PIV system, providing valuable insight into the flow dynamics at both micro- and macro-scales simultaneously. Our preliminary results have revealed interesting behaviors of the drying rate curve, which is significantly different from the traditional three-step process due to altered transport. We also observed that during the drying process, larger pores were depleted first, following which corner films and small pores were depleted, which can presumably be attributed to capillary pumping from large pores to small pores. The next steps will be to develop scaling laws to predict drying rate and quantify micro-macro-pore interaction based on the micro-PIV measurement.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS23 / 645

Local Equilibrium in Liquid Phase Shock Waves

Authors: Tage W. Maltby[1]; Bjorn Hafskjold[2]; Dick Bedeaux[3]; Signe Kjelstrup[4]; Øivind Wilhelmsen[5]

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Porous media can experience shock waves under certain conditions, for instance under ultrasound exposure 1. Shock waves are also observed in typical Hele-Shaw cells, during Haines jumps [2]. Modelling this is a vital part for understanding these complex phenomena. The question therefore arises; is it possible to use the governing equations for systems without shock waves; the balance laws and the constitutive equations, to model the fluid at the shock front? In this work, we consider the shock front in a liquid to examine the validity of non-equilibrium thermodynamic- and the hydrodynamic (Navier-Stokes) equations. In particular, we investigate the assumption of local equilibrium. Results from non-equilibrium molecular dynamics (NEMD) simulations are compared with numerical solutions of the Navier-Stokes (N-S) equations for supersonic shock waves with a Mach number near 2. The waves generated by the two types of simulations, travelled with nearly the same speed. The average absolute Mach-number deviation of the N-S simulations relative to NEMD was 2.6% in the considered time interval.

Five different methods to compute the surface excess entropy production were compared.
Three of the methods use the local equilibrium assumption as if the shock were a bulk system, and two of the methods assume local equilibrium between excess thermodynamic variables by treating the shock as a Gibbs dividing interface. The methods give excess entropy productions that are in excellent agreement, with an average deviation of 3.5% in the time-interval considered for the NEMD-simulations. For the shock wave studied in this work, we found that local equilibrium holds for the excess surface variables, but also for finer divisions of the planar wave. Our findings confirm the results we found by analyzing a shock wave travelling in a gas-phase [3], namely that local equilibrium holds for the excess surface variables and that local equilibrium is a good approximation for the bulk variables in the classical sense at the shock front also in the liquid phase. This can be regarded as a first step in the direction of computations of shock wave dissipated energy in porous media.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 648

Effect of Phase Change in Gas Diffusion Layer on Performance of a PEM Fuel Cell –a modelling study

Author: Grace Aquah[None]

Co-authors: Daniel Niblett ; Vahid Niasar [1]

[1] *University of Manchester*

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Research on the advancement and optimization of the PEMFC for commercialization centers around improving one or more of its limitations which include slow oxygen reduction kinetics, poor heat and water management, CO poisoning, and sourcing high-quality hydrogen as a fuel. Water management and subsequent improvement of oxygen reduction kinetics have been studied experimentally, numerically, and using computational models.
Several studies have proposed various options to improve the functioning of individual components of PEM fuel cells such as membrane coatings, catalyst type, gas channel shape (e.g., tapered), GDL microstructure, and as well as change of operating conditions. It has been proposed that regularly

ordered structures in a GDL will allow for smaller mass transfer loss and ohmic losses thereby improving the fuel cell performance 1. However, whether phase change (evaporation of water in GDL and condensation of vapor gas in GDL) can make a significant role in the efficiency of the PEM fuel cells is the question to be addressed in this study. In this study, using OpenFOAM coupled with the Volume of Fluid (VoF) method to simulate two-phase flow in the void space porous structure with and without phase change is simulated. The objective is to show the critical conditions when the phase change can have a detrimental role in the prediction of water management in GDLs.
References
1. Niblett, D.; Niasar, V.; Holmes, S. Enhancing the Performance of Fuel Cell Gas Diffusion Layers Using Ordered Microstructural Design. Journal of The Electrochemical Society 2020, 167, 013520.

Participation:

In-Person

References:

1. Niblett, D.; Niasar, V.; Holmes, S. Enhancing the Performance of Fuel Cell Gas Diffusion Layers Using Ordered Microstructural Design. Journal of The Electrochemical Society 2020, 167, 013520.

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Poster / 649

Near well bore formation damage by produced water reinjection

Authors: Maksim Kurbasov[None]; Karen Feilberg[1]

[1] *Danish Hydrocarbon Research and Technology Centre*

Corresponding Authors: klfe@dtu.dk, makur@dtu.dk

Objectives/Scope:
The oil industry produces large volumes of water along with the hydrocarbons (gas and oil), and in many cases the volumes of produced water exceeds the volume of water. Disposal of this contaminated water is a great challenge for the industry, however on fields where the wells are waterflooded with seawater an alternative disposal method is re-injecting the produced water. The major challenges with injectivity decline and formation damage during produced water re-injection are found in the near wellbore region. Deposits of schmoo, bacteria, production chemicals, oil components, scale and corrosion products are formed at the reservoir surfaces and will reduce the injectivity of produced water and seawater, containing dispersed components like solids and drops. Various well-stimulations are carried out without backflushing. The possible reasons for the reduced injectivity are thus formation of biofilms, clogging of the well with organic material from the produced water, both crude oil constituents and additives, salinity effects, temperature effects and particulates

among others. In addition, the filter cake development may happen as complete, "standard"matrix or partial blocking. This research proposes to investigate these effects by a novel combination of chemical analysis and core flood investigations, including injection experiments in a CT-scanner, to suggest improvement of produced water treatment for optimized water flooding with produced water.

Methods, Procedures, Process:

Flooding experiments through mini-cores or membranes will elucidate mechanisms such a pore blocking or cake formation through a combination of flow experiment, CT scanning and analysis of effluent composition. The smaller core or filter studies are less time consuming than longer core studies and are therefore well suited for screening filter cake development since this is independent of core length. . Analysis of the reservoir fluids and the injection effluents will be extended to include crude oil constituents and possible additives in the case of real produced water.

Results, Observations, Conclusions:
As a result of the conducted experiments, the processes are described, due to which the pore space is clogged inside the core samples. The dependences of the intensity of changes in the permeability of the rock and the elemental composition of the injected fluid are determined. Parallel studies were carried out using various methods, confirming the above theory.

As a result of the conducted experiments, the processes are described, due to which the pore space is clogged inside the core samples. The dependences of the intensity of changes in the permeability of the rock and the elemental composition of the injected fluid are determined. Parallel studies were carried out using various methods, confirming the above theory.

Novel/Additive Information:

This study will help extend the life of wells in the future. It will help to determine the reasons for the deterioration of the porosity properties of the reservoir and avoid further work to increase the permeability by increasing the characteristics of the injected water.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

650

Modeling the effects of pore-scale geochemistry on the performance of polymer and low salinity water flooding in carbonate reservoirs

Author: Angelo Kennedy Lino Limaluka[1]

Co-author: Yogarajah Elakneswaran [1]

[1] *Hokkaido University*

Corresponding Authors: elakneswaran@eng.hokudai.ac.jp, angelokennedy4@gmail.com

Abstract
Multi-phase pore-scale reactive phenomena involving crude oil, water and oil (COBR) generate physiochemical transformations to the petrophysical characteristics of the rock's porous interface and eventually influence the flooding process during oil and gas production. These interfacial reactions alter the interface's porosity, saturation, and permeability and either impede or improve the displacement and sweep efficiencies of water-based enhanced oil recovery (EOR) techniques. In low salinity waterflooding (LSWF) particularly, decades of previous studies report forms of these mechanisms as predominantly wettability alteration, multi-ionic exchange, and polar component desorption. However, despite extensive core-scale and field-scale studies on these mechanisms, limited reservoir-scale numerical models have incorporated the influence of geochemistry due to the illusive and microscale nature of these interactions. This has derailed and caused application hesitancy in the expansive use of LSWF even though it's a relatively arising and economical chemical EOR method that could improve harnessing of the overwhelming proportion of heavy oil in carbonate reservoirs, as well as light oil, by one-fifth. In this study, MATLAB Reservoir Simulation Toolbox (MRST) was integrated with a geochemical module (PHREEQC) to develop a model for up-scaling the role of these interfacial geochemical interactions for a more comprehensive simulation of polymer flooding and LSWF in carbonate oil formations. The LSWF's leading wettability alteration mechanism was included by the modification of the permeability parameter in the core and polymer modules of MRST. Then the performance of the model was validated through core-scale experimental results and was eventually used in the multidimensional assessment of the role of geochemistry in polymer flooding and LSWF. The simulation results demonstrate the synergy between low salinity and flood sweep efficiency of the injection phase, suggesting between 20-30% incremental oil recovery in these two techniques. Polymer flooding reduced water production by more than four-fifths and provided stability and extension of the production period. The results indicate a correlation between reservoir salinity and permeability heterogeneity/multilayering and the injection areal sweep efficiency.

Keywords: reservoir modeling, geochemistry, chemical EOR, MRST, PHREEQC

Participation:

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Energy Transition Focused Abstracts:

MS19 / 651

A domain decomposition strategy to compute effective electrical conductivity of large-scale 3-D digital rock images.

Authors: Rafael da Silva Vianna[1]; Ricardo Leiderman[1]; André Maués Brabo Pereira[1]

[1] *Institute of Computing, Fluminense Federal University*

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Electrical properties play an important role in the study of rock media. Estimating effective electrical properties of materials by means of laboratory testing is usually time-consuming and does not provide a complete understanding of the material microstructure. On the other hand, it is well known that numerical homogenization in conjunction with micro-computed tomographic images allows an efficient estimate of effective properties of heterogeneous materials in a non-destructive manner. For highly heterogeneous rock media, numerical homogenization requires large-scale models with high resolution images of Representative Volume Elements to obtain reliable results. These models often lead to simulations of very large linear systems of equations with billions of degrees of freedom, which require a large amount of computer memory to store data, quickly reaching its limit when simulating large volumes of material. In that sense, strategies to efficiently solve the systems of equations must be employed, e.g., the voxel-based (or image-based) meshing strategy, the Preconditioned Conjugate Gradient solver, and the Element-by-Element technique. However, even with such strategies for memory relief, memory allocation can still be an issue of concern. In addition, due to the memory-time trade-off, the application of those strategies demands tedious computations, and the solution may last excessively long. To solve these issues, Domain Decomposition Methods can be employed to accelerate the solutions and to solve larger-scale problems in cases of limited computer memory. In this work, we present a domain decomposition strategy in conjunction with image-based numerical homogenization to estimate effective electrical conductivity of highly heterogeneous rock media. We use the Preconditioned Conjugate Gradient method with a matrix-free strategy solving subdomain-by-subdomain to obtain the solution at the subdomains' boundary nodes. The data at internal nodes within each subdomain are condensed by solving a multiple right-hand side system with a Cholesky decomposition. We demonstrate that we can manage the memory and processing time by choosing an optimal number of subdomains. We validated our implementation by testing models that have analytical solutions and by comparing the results of a sample of sandstone obtained by our implementation and the open-source Julia package of numerical homogenization *chpack*. Furthermore, the presented methodology can be directly implemented in GPUs and clusters of CPUs to accelerate even more the numerical solutions.

Participation:

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Energy Transition Focused Abstracts:

Poster / 652

Micro-Scale Simulation and Characterization of Adsorption-Diffusion Behaviors of Nanoparticles onto Mobile Oil/Water Interface

Author: Can Ke[None]

Co-authors: Bin Yuan [1]; Yue Li

[1] *School of Petroleum Engineering, China University of Petroleum (East China)*

Corresponding Authors: lylzx0@163.com, upckecan@163.com, yuanbin@upc.edu.cn

A novel, hybrid pore-scale simulation method using Lattice-Boltzmann (LB) coupled with Langevin-Dynamics (LD) is proposed to investigate the physics of nanoparticles onto oil/water interface. Based on the LB method, the high-resolution characterization of oil-water two-phase interface is established, independent of further adjustment of interfacial tension (IFT), density and viscosity ratio. Then, in a fashion of discrete LB forcing source distribution, LD method is introduced to characterize the effects of Brownian motion, thermal fluctuation dissipation, multi-body hydrodynamics and particle-particle interactions. The new method is verified using the classical examples including Poiseuille flow velocity distribution calculation, wall wettability, Laplace equation, and the momentum decline of single nanoparticle. By the means of the new LB-LD coupling model, the adsorption and diffusion characterization of nanoparticles onto oil/water interface are investigated.
Moreover, by introducing the interference coefficient and non-equilibrium time, a modified Langmuir adsorption equation is first established by more accurately quantifying the adsorption characterization of nanoparticles and the consequent impacts onto the oil/water interfacial force, of which the classical Langmuir adsorption equation cannot take account. In addition, both the lateral and longitudinal diffusion coefficients of nanoparticles into the water phase and onto oil/water interface are obtained, and of which the underlying mechanisms are explained in detail. The correlation among the primary controlling factors including concentration, size and adsorption-diffusion of nanoparticles is well established. For a target representative example of SiO2 nanoparticles, it is observed that small size nanofluids with high concentration could accelerate the adsorption of nanoparticles and therefore help decrease oil/water interface tension. Attributed to the contributions of non-uniform flow field and curving effects of oil/water interface, the diffusion rates of nanoparticles onto oil/water interface are found as an exponential function of nanoparticle size. The novel simulation and characterization method provide valuable insights into how nanoparticles adsorb and diffuse onto oil/water interface that help reduce oil/water interface tension.

Participation:

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Energy Transition Focused Abstracts:

Poster / 653

Exploiting induced carbonate precipitation to improve reservoir storage integrity and geothermal system efficiency

Author: Philip Salter[1]

Co-authors: James Minto [1]; Katherine Dobson [1]; Jay Warnett [2]

[1] *University of Strathclyde*

[2] *NXCT National Centre for X-Ray Computed Tomography*

Corresponding Authors: j.m.warnett@warwick.ac.uk, katherine.dobson@strath.ac.uk, philip.salter@strath.ac.uk, james.minto@strath.ac.uk

Biomineralization, through microbially, thermally, or enzyme induced carbonate precipitation (MICP/TICP/EICP), is a naturally occurring and inexpensive cementation process that can seal microfractures and pore

throats that are inaccessible to cement and chemical based grouts. The porosity, permeability and thermal conductivity of porous geomaterials can therefore be controlled.

This project aims to determine the optimal compositional and injection parameters for biomineralization fluids in a range of subsurface applications relating to the low carbon energy transition. These include, improving the subsurface storage integrity of CO2 and H2 by reducing permeability around poorly sealed legacy wells, enhancing mineral trapping of geo-sequestered CO2, and improving the thermal performance of well casings and ground around low-high geothermal and thermal energy storage systems. We also assess the real time response of bio-cemented samples to harsh environmental conditions representative of those in the subsurface.

Understanding the interactions between geochemical reactions and the transport properties of fluid at the reservoir scale first requires biomineralization experiments to be carried out at the pore (micron) scale. These studies are essential for understanding principles of crystal formation, growth and hydrodynamic feedback mechanisms. Using real-time in situ x-ray computed tomography, the complex and synergistic factors involved in the biomineralization process can be better understood. Correlation of microstructural and macroscopic properties during repeated precipitation and dissolution events will allow refinement of larger scale reactive transport models that assess the suitability of different injection strategies.

Carbon Capture and Storage: The ability to create large, and spatially targeted low permeability regions could be a key tool in preventing leakage of geo-sequestered CO2 (and H2), as well as improving/restoring CO2 injectability and sweep efficiency. During 2-phase EICP a poor choice of injection angle and flow rate can inhibit the mixing of precipitation fluids, and therefore the efficiency of permeability reduction within a porous medium. The challenge of getting 2 fluids to mix uniformly in a tight pore space is only likely to get worse in high pressure, low permeability real world systems. We explore single-phase thermally-delayed, and pulsed EICP injection strategies that encourage better mixing within heterogeneous real-world systems. Injection cycles are repeated multiple times to target the larger (order of magnitude) reductions in permeability required to alter the flow behaviour of CO2 and other gases.

Thermal: Cement and bentonite based grouts typically have low thermal conductivities (<1 W/m K), which is detrimental to subsurface heat exchange. They often form a poor seal at the host rock/soil interface which can increase interfacial resistance. Minerals formed by MICP at the contacts between soil grains can greatly increase the thermal conductivity of the ground, particularly in unsaturated conditions. We explore enhancing this effect further with inclusion of highly conductive additives. For thermal energy storage applications specific heat capacity can also be increased with integration of phase change materials. By developing these specialized geothermal grouts/backfill, shallower boreholes may be required, greatly reducing cost.

The findings of this project have profound implications on the commercialization of engineered biomineralization, and its role in the subsurface energy transition.

Participation:

In-Person

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MS11 / 654

Gelation in model porous media investigated with environmentally-sensitive molecular rotors

Author: Romane Le Dizès Castell[None]

Co-authors: Elham Mirzahossein [1]; Marion Grzelka [2]; Daniel Bonn [1]; Sara Jabbari Farouji [1]; Noushine Shahidzadeh [3]

[1] *University of Amsterdam*

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Sol-gel processes have been widely used as an easy way to form stable thin films of inorganic polymeric materials for ceramics, coatings and more recently to enhance the mechanical properties of porous media. The latter is extremely important for the preservation of our stone cultural heritage, where several types of gel treatment have been proposed to consolidate damaged porous stones [1-3]. The consolidation treatment should not only restore the mechanical properties of the stone but also not change its physical appearance and other properties such as porosity or permeability. A homogeneous distribution of the gel in the porous network of the material is also very important, as fragile materials usually break at their weakest points. While the kinematics of transport and drying of Newtonian fluids in porous media have been widely studied by both experimental and theoretical approaches [4], the case of non-Newtonian fluids such as gels remains largely unexplored.

During sol-gel transitions induced by evaporation, the solution (sol) containing the precursor aggregates to form an elastic network that percolates throughout the material (gel) as the solvent evaporates. Here , we presents our study on the gelation dynamics in porous media: in capillaries as models for a single pore, and in quasi 2D 'lab-made'porous media with monomodal and bimodal pore size distribution [5]. By using molecular rotors (*i.e.* molecules whose fluorescence intensity depends on the local viscosity) the gelation dynamics have been investigated at the microscale [6]. This allows to estimate the local viscosity of the solution by doing fluorescence microscopy, and monitor the sol-to-gel transition. Confocal fluorescence microscopy then allows us to determine precisely where the gelation starts in the 2D porous media and how it evolves in time, because the fluorescence intensity can be directly related to the viscosity of the solution during the gelation.

In round and square capillaries, this technique allows us to investigate the impact of corner flows on the gelation kinetics and on the final distribution of gel. In the 2D model porous media, we observe that a heterogeneous gelation front appears near the evaporation boundary due to the advection. Our study reveals that a gradient of gel density develops starting from the evaporative boundary and successively invading the porous media, accompanied by a sharp decrease in the evaporation rate: the gel forms a 'skin'that decelerates the evaporation. The local viscosity of the solution during the drying can be successfully mapped with the molecular rotors and related to the decrease in the evaporation rate in capillaries and in 2D porous media with interconnected pores (see Figure).
Our results give new interesting insights into the sol-gel transition in confinement and the dynamics of gel formation in a porous network . Moreover, we show for the first time that fluorescent local viscosity probes are a promising new method to study the drying and transport of complex fluids in porous media without the need of highly advanced techniques such as as NMR imaging or X-ray microtomography.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 655

Dissolution-precipitation processes: patterns and product separation

Authors: Tomasz Szawełło[1]; Piotr Szymczak[2]

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We consider a porous medium infiltrated by a reactive fluid that triggers coupled dissolution/precipitation reactions at pore surfaces. To study these processes, we model the porous medium as a system of interconnected pipes (Budek, 2012) with the diameter of each segment increasing in proportion to the local reactant consumption. With this model, we investigate different growth regimes in an evolving porous medium, allowing for both erosion and precipitation of the dissolved material. We incorporate nucleation events and consider different models of reactive area evolution, including passivation processes on mineral surfaces. We benchmark the model against the experimental results of Poonoosamy et al. (2020) and then consider
the problem of separation of secondary reaction phases between small and large pores in the medium (Osselin, 2022), elucidating the underlying physical mechanisms.

Participation:

In-Person

References:

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Nanostructure and Interfacial Mechanical Properties of PEG/Cellulose Nanocomposites Studied with Molecular Dynamics

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The treatment with polyethylene glycol (PEG) is a widely used consolidation method to reinforce the decayed archeological wood structure1. We build composites composed of crystalline cellulose surrounded by PEG-treated amorphous cellulose matrix to represent a simplified model of wood S2 cell wall layer with PEG treatment. Pullout test simulation are used to reveal the impact of PEG treatment on the interfacial mechanical properties of the fiber-matrix composite at atomistic level.
GROMACS package [2] and the OPLS force field [3] are used for molecular dynamics simulations. The composites in the dry state are composed of an infinitely long crystalline cellulose fiber embedded in a PEG-impregnated amorphous cellulose matrix. By randomly inserting water molecules into the porous region, moisture content levels are gradually increased. The whole set of samples spans 7 levels of PEG ratio and 11 levels of moisture content resulting in an extensive parametric study in terms of both PEG and moisture content variations.
At equilibrium, the nanostructure of all composites is thoroughly probed. PEG replaces the amorphous cellulose around crystalline cellulose proportional to the overall PEG ratio, which shows PEG molecules form a mixture with the amorphous matrix. Crystalline cellulose significantly impacts the distribution of the matrix and the hydrogen bond formation between crystalline cellulose and the matrix is a key factor in studying this interface behavior. Water molecules are found to not only soften the matrix, but also act as a lubricant between crystalline cellulose and the matrix. The total number of hydrogen bonds formed between crystalline cellulose and the matrix increases with higher PEG ratio, which is considered at the origin for PEG consolidating the interface.
The curve of shear force versus relative displacement of crystalline cellulose with matrix, reflects the stick-slip movement of the fiber during the pullout test. The number of hydrogen bonds closely follow the stick slip curve implying a strong correlation between shear force and hydrogen bond network at the interface. The maximum shear stresses are extracted, and the highest value happens at 3%-6% moisture content, which show the consolidation of the interfacial mechanical property by PEG at this moisture content range comparing with the dry states.
Based on the simulation data, a shear force model based on number of hydrogen bonds is developed. The assumption that the shear force is resulting from the hydrogen bonds between the fiber and the matrix is validated. The model shows that the shear stress provided by per hydrogen bond between crystalline cellulose and PEG is lower than the shear stress provided by per hydrogen bond between crystalline cellulose and amorphous cellulose. However, this lower value for the PEG mixture is partly compensated by an increase of total number of hydrogen bonds. This study can improve the understanding of the fundamental mechanisms by which PEG-treatment strengthen archeological wood at the molecular level.

Participation:

Online

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Energy Transition Focused Abstracts:

Poster / 658

Compositional and Structural characterization of complex fluids via Electrical Impedance Spectroscopy and Electron Microscopy

Authors: Nicolae Tomozeiu[1]; Hélder Marques Salvador[2]; Hamid Mansouri[2]

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The water-based inks with polymeric latex particles used in printing technology deliver prints of superior quality at a low cost and environmental friendly. Via ink formulation and drying processes, the inkjet prints are characterized by a wide color gamut, intense gloss with tonal graduations and excellent mechanical properties.

Various methods and techniques are used to investigate the constituents of water based inks bridging the ink formulation to the print final product. In this work we propose the use of Electrical Impedance Spectroscopy (EIS) method with a cylindrical measurement cell in combination with Electron Microscopy (HR-SEM). The EIS is used to characterize, from simple towards complex mixtures, fluids from resembling the water-based ink. Particles like pigment and polymeric latex are components of such complex fluids. In this work we use EIS to study material properties (e.g. dielectric constants, and electrical resistivity) of complex mixtures and, based on a calibration procedure, to identify the composition of the mixture. From here, physical processes such as water evaporation of aqueous mixtures, have been investigated in their dynamics.

The hardening of the complex mixtures with particles allowed us, via HR-SEM, to investigate the structural properties of the resulted ink layer as a function of the initial composition.

Theoretical models and computational simulations were used to analyze the EIS experimental data and to improve our understanding.
We consider the EIS in combination with microscopy a valuable tool in these studies; of course there are limitations of the method, which together with its advantages, are the discussed in this work.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 659

Deep Learning-based inverse modeling of a tank model of a channelized aquifer

Authors: Vanessa A. Godoy[1]; Valeria Todaro[2]; Gian F. Napa-García[3]; Andrea Zanini[2]; J. Jaime Gómez-Hernández[3]

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Inverse modeling plays a fundamental role in the subsurface characterization of aquifers, given the scarcity of available data. Several techniques have been proposed in the literature and tested using synthetic examples. However, one of the big criticisms of these techniques is the lack of demonstrations in real cases. In this context, this study presents the application of two of the most advanced inverse modeling techniques: the Ensemble Smoother with Multiple Data Assimilation (ES-MDA) and Deep Learning-based inverse modeling (DL), for the characterization of the non-Gaussian hydraulic conductivity field of a 2D tank model of an aquifer. The experiment consisted of the release of a fluorescent solution from a point source on a horizontal flow field (constant head imposed to the left and right boundaries of the model). The physical model was built with glass beads of two sizes, forming a homogeneous low hydraulic conductivity matrix with sub-horizontal high conductivity channels embedded. The inverse problem pursued the identification of the hydraulic conductivity from measurements of the solute concentration at given locations and times. Prior field realizations were generated using multiple-point geostatistics to resemble the channel patterns observed on the physical model. The efficiency and accuracy of both techniques in terms of computational time and error/dispersion in hydraulic conductivity and solute concentration are evaluated.

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Energy Transition Focused Abstracts:

660

Numerical Investigation of Multiple Influential Factors in Hydraulic Fracturing Processes Using Coupled Discrete Element-Lattice Boltzmann Method

Authors: Weiwei Zhu[1]; Zhiqiang Chen[2]; Moran Wang[1]

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Hydraulic fracturing refers to the process of injecting highly-pressurized liquid into a well to break up bedrock formations, which is vastly implemented in stimulating unconventional reservoirs, e.g. shale oil, shale gas, and enhanced geothermal systems (Gandossi & Von Estorff, 2013). Many factors can influence the geometry of hydraulic fractures, like formation parameters (e.g. in-situ stress), treatment parameters (e.g. injection rate and fluid viscosity), and rock properties (e.g. rock strength heterogeneity and formation permeability) (Chen et al., 2020; Duan et al., 2018). However, a systematic and comprehensive investigation of the influential factors and their coupled effects on the hydraulic fracturing process is rarely conducted.

In this research, a discrete element-lattice Boltzmann method is implemented to simulate the hydro-mechanical behavior in a hydraulic fracturing process (Galindo-Torres, 2013， Chen & Wang, 2017). Different influential factors, including injection rates, fluid viscosity, in-situ stress states, heterogeneity of rock strengths, and formation permeability, are considered and their individual and coupled impacts on the initialization and propagation of hydraulic fractures are evaluated.

We simulate a rectangular domain with a constant flow-rate condition for the inlet (left side) and a fixed pressure is assigned on the right side of the domain. All the other boundaries are set as solid. Different parameters are selected to characterize the different influential factors. We conduct a Buckingham analysis to scale simulation parameters (injection rate and in-situ stress magnitude) with parameters in actual experiments. The shape factor (m) in the Weibull distribution is used to characterize the heterogenous bond strengths for brittle rocks. An infinitely large m corresponds to a homogeneous structure, while a low value of m indicates a heterogeneous structure. The solid fraction ratio \gamma in an immersed boundary method is used to characterize the formation permeability. A larger \gamma indicates a less permeable formation.

In the first stage, we test the individual effect of each factor on the initialization and propagation of hydraulic fractures. From preliminary observations, several conclusions are listed below:

i. All factors have a significant impact on the fracture initialization pressure. A higher injection rate, higher viscosity, and larger in-situ stress will increase the initialization pressure, while a higher formation permeability and higher heterogeneity degree of bond strengths will decrease the initialization pressure.

ii. Injection rate and heterogeneity degree have much significant impact on the complexity of generated fractures. Fluid viscosity, in-situ stress states, and formation permeability do not change the geometrical complexity.

iii. Hydraulic fractures are usually tensile fractures, however, they usually do not have pure tensile displacement. Shear fractures are possible and the shear displacement can be significant under certain conditions, such as a high injection rate, and high heterogeneity degrees.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS07 / 661

Resonance, Rayleigh Flows and Thermal Choking: Convective Electromagnetic Energy Harnessing from Absorbing Porous Media.

Authors: Burt Tilley[1]; Vadim Yakovlev[1]; Ajit Mohekar[1]

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Electromagnetic (EM) Heat Exchangers (HX) are systems which convert EM energy into heat or mechanical work. One potential design consists of a porous lossy ceramic material heated by EM waves saturated with a compressible gas coolant. EM heating of ceramics is nonlinear, since the loss factor is temperature dependent. Designing such EM HXs requires an understanding of the coupling between temperature, the electric field, and gas dynamics at the pore scale. To mimic this microscale phenomena, a single channel with a high-speed gas coolant in perfect thermal contact with a thin solid ceramic layer is considered, with an applied plane-wave electric field propagating normal to the channel walls. From a thin-domain asymptotic analysis, the conservation laws reduce to a Rayleigh flow in the gas coupled with averaged thermal energy conservation equations at leading order. The kinetic energy of the gas increases about 10 times the inlet value when thermal runaway occurs in the ceramic region, and thermal choking is possible when the coolant reaches the sonic state. Extensions to high-speed flows in ceramic porous media are discussed. This work was supported by a grant from the US Air Force Office of Scientific Research (AFOSR) award FA9550-18-1-0528, for which the authors are grateful.

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In-Person

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MS01 / **662**

The effect of mixed convection and hydrodynamic dispersion on CO2 dissolution in saline aquifers

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One of the most important trapping mechanisms in CO2 geologic storage is convective dissolution. When CO2 is dissolved, it slightly increases the brine density, resulting in natural convection in the form of dense fingers. In most previous studies, natural groundwater flow and the associated hydrodynamic dispersion were neglected. In this work, we study the effect of hydrodynamic dispersion and natural and forced convection (mixed convection) on CO2 dissolution.
We use laboratory-scale analog experiments and numerical simulations to study the influence of horizontal flow and hydrodynamic dispersion on the fingers morphology and dissolution flux. The results indicate that background flow and dispersion significantly reduce the fingers wavenumber and velocity. Yet, the effect on the dissolution rate is complex and non-monotonic. Based on the simulated results, new scaling laws that predict the dissolution rate and wavenumber in the presence of dispersion and background flow were developed. These new laws show that the available predictions in the literature overestimate the dissolution rates in potential storage sites.

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MS06-B / 663

Drainage pore-invasion patterns in porous media: role of interfacial dynamics

Authors: Mahdi Mansouri-Boroujeni[1]; Cyprien Soulaine[1]; Mohamed Azaroual[2]; Sophie Roman[3]

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Immiscible two-phase flow through porous media is composed of a series of pore invasions; however, the consequences of pore-scale processes on macroscopic fluid front behavior remain to be clarified. In this work, we perform an analytical and experimental investigation of front behavior and pore invasions dynamics during drainage for various viscosity ratios and capillary numbers. We use a microfluidic setup made of a pore-doublet geometry to isolate and explore pore-invasion mechanisms. We apply a model based on volume-averaged Navier–Stokes equations to capture interface dynamics. Different invasion mechanisms are characterized and correlated with front behavior for various flow conditions. For the viscous flow regime a succession of continuous pore invasions is observed, leaving a thick layer of wetting phase behind at pore curvatures. Abrupt interfacial jumps, followed by an apparent stagnant condition of the interface, are observed for the capillary flow regime. We identified a new regime, called crossover flow regime, for which pore invasion shows a mixed behavior between capillary and viscous dominated regimes. The global front behavior is predicted based on the numerical simulation and experimental results for all flow regimes.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS09 / 664

Improved Amott Experiments Capture Dynamics of Spontaneous Imbibition into Mixed-Wet Carbonate-Rock with Non-Zero Initial Brine Saturation

Authors: Ksenia Kaprielova[1]; Maxim Yutkin[1]; Ahmed Gmira[2]; Subhash Ayirala[2]; Ali Yousef[2]; Clayton Radke[3]; Tadeusz Patzek[4]

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Spontaneous imbibition of brine at nonzero initial water saturation is an important mechanism for recovering crude oil from mixed-wet heterogeneous carbonate rock. Many studies focus on studying or modeling spontaneous imbibition of brine into fully oil-saturated (i.e., without connate water) or water-wet porous media. As a result, adequate models describing spontaneous imbibition process into rock with nonzero initial water saturation and mixed-wettability do not exist.

First, we review the experimental variables that are important for spontaneous imbibition in water-wet and mixed-wet rocks in the presence of connate water. We show that the classic Amott experiment, broadly used to evaluate ultimate oil recovery, masks several flaws that hinder the interpretation of recovery dynamics and thus the development physical and predictive recovery models. The key aspects are 1) contribution of the buoyancy-driven oil production; 2) wettability-dependent oil hold-up at the core surface; and 3) inconsistent outer surface wettability of mixed-wet limestone core plugs.

We then modify the classic Amott testing procedure to minimize experimental artifacts in the recovery dynamics. The main modifications include the following: 1) capping the top and bottom faces of core plugs with glass discs to eliminate the axial flow and enforce only 1D radial two-phase flow; 2) continuous shaking throughout the entire experiment to eliminate the oil external-surface hold-up with different core wettability states; 3) degassing of both brine and oil prior to any experiments. We show that the modified Amott experimental procedure obtains smooth and reproducible oil-recovery histories for oil-saturated core plugs with different wettability conditions of limestone rock. Figure 1 compares the cumulative oil recovery versus square root of time in the classic Amott test and with the introduced modifications. Note the smooth oil recoveries compared to the classic procedure.

Finally, we show that the resulting smooth recovery profiles of oil production can be described by a statistical model that fits the data very well. For the first time, we demonstrate that generalized extreme value (GEV) distribution can be applied to model spontaneous brine imbibition into water-wet and mixed-we cores in the presence of connate water. Figure 2 is an example of the GEV scaling of cumulative recovery versus square root of dimensionless time for water-wet core plugs.

The next step in developing our new approach to modeling spontaneous imbibition in the presence of connate water is to elaborate on how the distinctions of the physical processes during oil recovery by spontaneous imbibition are reflected by the GEV statistics. We believe, that our GEV modeling approach will serve as a foundation for the development of a next-generation predictive model of oil-recovery dynamics from mixed-wet carbonates.

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Energy Transition Focused Abstracts:

MS06-A / 665

Two-phase non-linear flow in Pore Network Model

Author: Federico Lanza[1]

Co-authors: Alex Hansen [2]; Laurent Talon [3]; Alberto Rosso [4]; Andreas Hennig [5]; Santanu Sinha [6]

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Immiscible displacements in porous media have been extensively explored, both experimentally and numerically, in the last decades, and, for two-phase Newtonian flows, it was shown that the competition between the characteristic forces involved, like viscous and capillary forces, determines the structure of the invasion pattern 1. In this work, we try to extend these studies taking into account some non-linear behaviors, namely the presence of yield stress and the formation of compact displacement regions. If the displaced fluid consist in a non-Newtonian Bingham liquid, flowing like a Newtonian fluid only above a finite stress, a yield stress dominant pattern emerges, characterized by needle-like paths of low dimensionality [2]. On the other hand, compact invasion regions, in which every pore is invaded by both fluids in a rapid succession, emerge when imposing a constant pressure drop throughout the medium, as recently shown experimentally in a porous Hele-Shaw cell [3]. We perform numerical simulations of a two-dimensional porous medium, in the framework of the dynamical Pore-Network model [4]. An algorithm, part of the Augmented Lagrangian methods class and already implied successfully for the study of non-Newtonian flow, was adopted for solving the non-linear relation between the flow rate and the pressure at the pore level [5]. We then characterize the structure of the invasion patterns related to these non-linear effects, measuring quantities like the saturation of the invading phase and the fractal dimension of the corresponding paths, and comparing these values with the ones present in literature for the two-phase fully-Newtonian flow. The domains of validity of these patterns are finally mapped onto a plane with axes the ratio between the different forces into play, obtaining a 'phase-diagram' for these immiscible invasion displacements.

Participation:

In-Person

References:

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Nanoparticle migration in a porous medium and a polymeric inelastic non-Newtonian fluid

Authors: Masoud Babaei[1]; Takshak Shende[2]; Vahid Niasar[1]

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Subsurface applications, such as soil remediation and increased oil recovery, need precise control of the diffusion of nanoparticles in polymer solutions via porous media. The non-Newtonian behaviour of polymer solutions, the Brownian motion of nanoparticles, and the spatial heterogeneity of porous media all have an impact on dispersion. In this work, we employ the Euler-Lagrangian approach to study the transport of nanoparticles and inelastic non-Newtonian fluids (represented by the Meter model) via various porous medium samples and injection rates. Dispersion of nanoparticles in the porous media is shown to exhibit non-Fickian behaviour, indicating that their velocity distribution is not Gaussian. Dispersion of nanoparticles along both the longitudinal and transverse axes is also facilitated by their Brownian motion.

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MS15 / 668

CNN model for multi-component digital rock modeling based on CT and QEMSCAN images

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The types, content changes and distribution of mineral components in unconventional reservoirs are complex and diverse, which brings great difficulties to reservoir evaluation. In order to more accurately carry out numerical simulation of rock physical properties based on digital cores, it is necessary to accurately identify and divide the skeleton, establish multi mineral 3D digital cores, and determine the types and distribution forms of each mineral component. The image multi-threshold segmentation of grayscale core images is a common method to obtain multi-component core images, but the thresholds need to be manually adjusted, which is time-consuming and may cause large errors. This study reveals the application advantages of semantic segmentation method in digital core, and establishes a multi mineral 3D digital core automatic semantic segmentation model based on depth learning. Firstly, the mineral distribution characteristics in the study area are obtained through QEMSCAN and the typical mineral types are determined. Secondly, it is proposed to use the

typical mineral (glauberite) in the study area for feature similarity analysis to achieve automatic and accurate image registration. Then, the sample data is determined by image alignment, interpolation, image filtering, brightness averaging, sharpening and other preprocessing methods. Finally, a multi mineral 3D digital core semantic segmentation model based on depth learning is established. The obtained multi mineral 3D digital core is highly consistent with the QEMSCAN mineral analysis results, retaining the layered distribution of shale minerals, and is applied to conductive simulation and electrical property research.

Participation:

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MS06-B / 669

Surface relaxivity and its role in permeability prediction

Authors: Ricardo Leiderman[1]; Alexsander Cunha[2]; Rafael da Silva Vianna[None]

Co-authors: Pedro Vianna [1]; André Souza [1]; Pedro Cortez Lopes [1]; André Maués Brabo Pereira [2]; Rodrigo Bagueira [1]

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In the limit of the so-called fast diffusion regime, the solid-fluid interaction plays the major role in the Nuclear Magnetic Resonance (NMR) transverse relaxation phenomenon, and the saturating fluid characteristic transverse relaxation time (T2) is inversely proportional to the surface-to-volume ratio (S/V) of the pore where it resides 1. The surface relaxivity (ρ), a parameter that characterizes the strength of relaxation induced by the solid/fluid interface, is the proportionality constant that relates T2 to S/V. In that sense, when an estimate for ρ is available, the T2 distribution (a distribution of characteristic relaxation times) can be converted into a S/V distribution straightforwardly. Indeed, the more accurate we estimate ρ, the better we estimate the S/V distribution and, therefore, the better we estimate all the subsequent related petrophysical deliverables [2]. We explore this notion in the present work, within the context of Machine Learning. To do that, we divided the study into three parts: In the first part, we used an in-house developed Random Walk implementation to simulate the T2 distribution in a large collection of in-house generated 3D digital rocks, using a single value for ρ. In addition, for the same collection of digital rocks, we estimated the absolute permeability with the aid of an in-house developed Voxel-Based Finite Element implementation. We then trained and tested a Random Forest Machine Learning model for estimating the permeability from the T2 distribution using the 10-fold Cross Validation protocol. The second part of the study was analogous to the first one, but this time we used several rondomly-chosen different realistic values for ρ, one for

each rock, to simulate the T2 distributions. Then, we trained and tested again the Machine Learning model for estimating the permeability from the T2 distribution using, once more, the 10-fold Cross Validation protocol. The third part of the study was similar to the second one, except that, now, we added one more stage in the workflow: for each rock, using the value of ρ used to simulate its T2 distribution, we converted the T2 distribution into a S/V distribution. We did that for the entire rock collection. Then, we trained the Machine Learning model for estimating the permeability from the S/V distribution (instead of the T2 distribution). We compare the success rate for the three cases and show that it is high and practicaly the same for the first and third parts of this work, but lower for the second part.
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Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS10 / 670

Zoom-tomography applied to diverse porous media research at the MOGNO beamline from Sirius synchrotron

Authors: Nathaly Lopes Archilha[1]; Talita Rosas Ferreira[1]

Co-authors: Victor R. M. Zelaya [1]; Daphne Silva Pino [1]; Bruno B. Kerber [1]; Murilo Carvalho [2]; Paola Cunha Ferraz [1]; Larissa Macul Moreno [1]; Otávio Moreira Paiano [1]; Eduardo Xavier Miqueles [1]

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Synchrotron light sources present advantages over laboratory-based X-ray Computed Tomography (XCT) in terms of spatial and temporal resolution. The reasons are the smaller size of the X-ray source and the higher photon flux generally achieved in particle accelerators. In this context, Sirius, the Brazilian 4th generation light source, will count on a world-leading micro and nano X-ray

imaging beamline, MOGNO, which will be focused on time resolved and multi-scale experiments (Archilha et al., 2022). The project of MOGNO has been presented at InterPore in 2018, before its construction had started. Now, after five years, the goal of this work is to present the current status of MOGNO and recent imaging of diverse examples of porous media using the cutting-edge zoom-tomography capability that has recently been validated.
The cone beam geometry of MOGNO covers up to 27 meters between the sample and detector, enabling continuous magnification of the image, also known as zoom-tomography. This beamline will be equipped with a direct area-detector that provides a maximum field of view (FOV) of ~85x85 mm2. At this maximum FOV, the sample is positioned close to the detector and the image resolution is 55 μm, which is limited by the pixel size of the detector. By moving the sample towards the X-ray source, specific regions of interest inside the sample can be selected with smaller FOVs down to ~150 μm and higher image resolutions up to 120 nm, which is limited by the projected size of the X-ray beam focus. However, the maximum FOV for a given experiment must respect the X-ray transmission dependency on the sample chemical composition. In this regard, MOGNO works in tender (22 and 39 keV) and high (67.5keV) X-ray energies, which makes it a versatile beamline that can be used to image a diversity of materials, ranging across rocks, soils, plants, fossils, biological tissues, etc.
The zoom-tomography capability is on the spotlight as this will considerably benefit the currently represented research areas at MOGNO, such as geological, biological, material, earth/planetary, agriculture, and archeology (e.g., Moraes et al., 2022; Ferreira et al., 2022). These areas have in common the hierarchical nature of the materials. Therefore, we propose to show real examples of zoom-tomography at the MOGNO beamline applied to different porous media, for instance, of pre-salt reservoir rocks, roots growing in soil, plant stem, bone regeneration, fossil, and biological tissues. These samples attenuate the X-rays differently and thus impose different challenges in the image reconstruction, requiring robust computational methods capable of working with both light and hard samples, at times including phase retrieval algorithms. We expect to show opportunities for studies that can already be performed at this beamline, which will be open for scientific commissioning with external users in 2023.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

671

Nanoconfined water and aqueous solutions investigated by molec-

ular simulations and NMR

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The dynamic and thermodynamic properties of a fluid confined within nanopores differ from its bulk properties. Molecular Dynamics Simulations (MDS) are powerful tools to study such confinement-induced phenomena, particularly when combined with experiments. For instance, the relaxation times (T1 and T2) probed by Nuclear Magnetic Relaxation Dispersion (NMRD) methods can be extracted from both experiments and simulations, and compared without adjustment parameter.
Here we use MDS and NMRD to study the dynamics of water within slit nanopores, including nanopores made of salt. We explore large ranges of surface charge, hydrophilicity, and roughness and their respective effects on the dynamics of the water by extracting the NMR relaxation time T1. We correlate our results with the structuring and average orientation of the water molecules near the solid surfaces. We then derive a model based on first passage time to relate the successive adsorption/desorption of the water molecules with the NMR relaxation time T1. Overall, our study help bridge NMR relaxation measurements with the dynamics of water in confinements.

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Energy Transition Focused Abstracts:

MS21 / 672

Understanding pre-Darcy flow and velocity-dependent permeability in porous rocks through neutron imaging

Authors: Fernando Vieira Lima[1]; Stephen Hall[1]; Erika Tudisco[1]; Jonas Engqvist[1]; Robin Woracek[2]; Stefanos Athanasopoulos[2]; Philip Vestin[1]; Jan Hovind[3]

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Darcy's Law is a classic example of a scientific paradigm in the study of fluid migration through porous media. However, many authors have reported deviation of flow regimes from Darcy's law at low flow velocity 1 when analyzing fluid flow in rocks, often called pre-Darcy flow. In addition

to the velocity dependence of rock permeability, the heterogeneous nature of geomaterials deserves equal attention when analyzing the hydraulic behavior of rock masses. When performing conventional permeability tests, little is known regarding fluid behavior within the sample. In this context, neutron imaging provides an ideal full-field technique for better understanding these phenomena. This work employs neutron imaging to investigate the influence of sample heterogeneity and flow rate on flow paths and permeability by performing flow tests with Idaho Gray sandstone cores.
In-situ experiments were performed at the Neutra instrument at Paul Scherrer Institut (Switzerland) using the setup described in Vieira Lima et al. [2]. The flow tests were carried out on samples saturated with heavy water (D2O) or normal water (H2O) by pressure-driven percolation of the respective opposite fluid. Before the neutron experiments, x-ray tomograms were acquired to provide a reconstructed 3D image with a cubic voxel width of 13 μm for a detailed characterization of the pore and grain structures. During each test, neutron radiographies were acquired with an exposure time of 1 s, generating 2D images with a 200 μm pixel size. The difference in neutron attenuation between D2O and H2O was exploited to track the advance of the infiltration front; as D2O and H2O are otherwise very similar fluids, a near single-phase fluid condition was assumed. Boundary fluid flow-rate and pressure measurements were recorded and correlated with the images. The raw neutron images were processed using in-house python codes, generating maps of saturation-time and -degree plus flow-speed fields. 3D porosity fields and pore network models (using Porespy software [3]) were generated from the x-ray tomograms. Simulations of the visualized phenomena were performed using the "Invasion Percolation"and the "Stokes Flow"algorithms from the OpenPNM package [4] based on the 3D pore networks.
Pre-Darcy flow was observed from the boundary measurments in all samples (Fig.1) with a reduction in the bulk permeability with the flow rate. The results from the neutron radiography in the form of 2D maps of the flow-field evolution showed that the percolation followed preferential paths due to the natural heterogeneity of the samples (Fig.2), which could be correlated with the heterogeneity in the porosity fields (Fig.3). In the injection of either of the percolating fluids (H2O and D2O), the flow rate increase generated a flattening of the advancing flow fronts and reduced spatial heterogeneity of the infiltration, indicating that more pores were accessed at higher injection rates and suggesting threshold rates/pressures exist to access different parts of the pore network. The simulations of the fluid infiltration using the pore network models reproduced well the observed flow patterns and showed a good performance in predicting the change in bulk permeability for each flow rate.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 673

Forward and Inverse Modeling of Nonisothermal Multiphase Poromechanics using Physics-informed Neural Networks (PINNs)

Authors: Ehsan Haghighat[None]; Danial Amini[1]; Ruben Juanes[2]

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Solving the inverse problem (identifying the parameters of PDEs) typically poses exceptional challenges due to the nonlinear nature of the governing equations, their strong coupling, and the extremely high dimensionality of the problem. Classical data assimilation and optimization techniques treat forward solvers as black-box estimators and therefore typically require an unfeasible number of forward simulations during the optimization. Physics-informed neural networks (PINNs), developed to extend the inherent capabilities of artificial neural networks to incorporate PDE constraints (Raissi et al., JCP 2019), offer the potential of a unified forward and inverse solver, and thus a framework to inherently combine measured data and model predictions. Here, we develop such a framework for forward and inverse modeling of thermo-hydro-mechanical (THM) problems using PINNs.

While PINNs have received exponentially increasing attention in recent years since their advent in 2019, their application to forward and inverse modeling of multiphysics problems remains challenging. In our experience this is because, when the physical processes are strongly coupled, network training is fragile and slow. In our recent works (Haghighat et al., CMAME 2021, Amini et al., JEM 2022), we proposed a sequential training strategy for the forward solution of HM and THM processes in porous media. Here, we build on these previous studies to develop a strategy for the solution of the inverse problem. To this end, we propose a revised nondimensionalization of the THM formulation that is more suitable for inverse problems. We validate the algorithm on benchmark porous media problems, including Terzaghi's consolidation problem, Barry-Mercer's injection-production problem, and consolidation under non-isothermal partially-saturated conditions. Although we use synthetic data to validate our algorithm, we restrict the total number of sensors to a very small number. Our results show the applicability of the PINN approach for inverse modeling of THM processes, thus paving the way for the application of PINNs to inverse modeling of complex nonlinear multiphysics problems.

Participation:

In-Person

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Poster / 674

Delineating external stressor signals as time-variant conditions affecting DNAPL source zone formation

Author: Christian Engelmann[1]

Co-authors: Helen K. French [2]; Kaveh Sookhak Lari [3]; Charles J. Werth [4]; Traugott Scheytt [1]

[1] *TU Bergakademie Freiberg, Chair of Hydrogeology and Hydrochemistry*

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Groundwater aquifer systems serve as a major source of drinking and irrigation water supply. In recent years, they have also become valuable for geothermal energy applications. The protection of groundwater against detrimental factors is crucial to preserve this valuable water supply and ensure a sustainable energy transition. Subsurface contamination by dense non-aqueous phase liquids (DNAPLs) can cause adverse effects for humans and the environment. These organic compounds are omnipresent in industrialized and developing countries, particularly in areas with energy production (e.g., oil and coal industries, chemical plants), industrial fabrication (e.g., steelworks, wood impregnation) and transportation hubs (e.g., railway systems, roads, airports). Once re-leased into soils, DNAPLs form slowly miscible source zones that can contaminate groundwater for decades.
Despite a range of existing subsurface remediation techniques, mostly for economic reasons, natural attenuation of aqueous DNAPL components in groundwater represents the most commonly applied cleanup option. As a con-sequence, the fate of contaminated sites remains unclear due to insufficient data and knowledge of DNAPL source zones. Climate change and anthropogenic activity may jointly add new hazard potentials by inducing hydraulic and thermal stressors potentially affecting present and emerging source zones. A robust understanding of the processes associated with DNAPL source zone formation under changing conditions is therefore crucial to ensure an efficient assessment of contaminated sites.
Our current research aims at systematically investigating the transient dynamics of DNAPL source zone formation, and employs experimental and model-based methodologies to evaluate the relevance of changing external stressors (hydraulic, thermal) compared to subsurface and fluid phase properties. In this study, we present a methodology to systematically delineate variation signals, necessary for the definition of boundary conditions in models considering changing conditions, from multi-scale field site information (e.g., monitored time series). For this, a range of field sites under variable anthropogenic pressures showing different intrinsic hydro(geo)logical characteristics are involved.

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In-Person

References:

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Poster / 675

Pore size distribution and permeability improvement estimation of porous rocks: a comparison of image-based methods and experimental NMR measurements

Authors: Ricardo Leiderman[1]; André Maués Brabo Pereira[2]; Jefferson Filgueiras[1]; Andre Souza[1]; Rodrigo Bagueira[1]; Francisco Benavides[1]

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The knowledge of pore size distribution and absolute permeability of porous media are key for a proper petrophysical characterization of a reservoir, which directly impacts the accuracy of hydrocarbon reserves estimation and the production strategies optimization. For the Oil and Gas exploration industry, downhole measurements are done to infer several properties and to perform a formation evaluation based on petrophysical analysis and interpretation of such data. Among them, Nuclear Magnetic Resonance (NMR) is becoming a key logging tool since it is sensitive to the saturating fluids only, i.e. it is not affected by the matrix minerals. Hence, it is ideal for the direct determination of porosity, for example. The main application of NMR on porous media study is based on the measurement of a magnetic relaxation process of the fluid´s nuclear spins, in this case those from the hydrogens that constitute the hydrocarbon chains and the formation brine. Such relaxation process, in porous media, is proportional to the pore sizes and to a parameter called surface relaxivity, which scales the intensity of the matrix-fluid interaction. Hence, to a proper characterization of pore sizes based on NMR relaxation measurements, surface relaxivity must be properly determined 1.

In this work, we formulate and solve an inverse problem to obtain the suface relaxivity parameter as a function of pore sizes for 14 sedimentary rock cores: 7 sandstones and 7 carbonates. In this methodology, micro-tomographic images of the rock samples are the input for simulations that applies Random Walk (RW) and a genetic algorithm to infer a surface relaxivity function that varies with the size of the pores. Hence, a distribution of pore sizes can be obtained from this function when correlated to experimental NMR data measured from the same samples.

Using NMR data, absolute permeability is modeled as a linear product of porosity and the mean relaxation time value, i.e. NMR data is used as a proportionality parameter to the pore sizes [2]. Applying the inverse problem developed here, the pore size mean value can be calculated with higher accuracy, with also increased the absolute permeability prediction. The estimated absolute permeability results were compared to experimental data measured from the same samples.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 676

Modelling Long-Term Thermal Energy Storage in Water-Gravel-Filled Artificial Basin Systems

Author: Christoph Bott[1]

Co-authors: Christoph Trinkl [2]; Mathias Ehrenwirth [2]; Abdulrahman Dahash [3]; Peter Bayer [1]

[1] *Martin Luther University Halle-Wittenberg, Institute of Geosciences and Geography, Applied Geology*

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With the growing prevalence of renewable energy sources in innovative energy systems, interactions between energy supply and demand become more dynamic and complex. Therefore, along with the deployment of efficient and low-emission energy sources and sinks, energy storage is a central element of the energy transition. Especially for the case of thermal energy, a mismatch between high energy supply and low demand in summer and vice versa in winter is striking—resulting in a critical demand for seasonal solutions.

In the past, various concepts were established for large-scale, sensible, low-temperature applications. Closed systems (tank and pit thermal energy storages) have been developed as site-independent solutions, differing in their constructional design with different building components. Further, water-gravel thermal energy storage (WGTES) feature a water-saturated matrix filling (i.e., gravel, sand) with an indirect charging and discharging system (usually multi-level piping loops). Among the closed concepts, WGTES is considered the most complex variant, which simultaneously offers less maximum storage capacity due to a reduced effective volume. In addition to the resulting sophisticated internal thermal behavior, a number of additional components (sealing, insulation, static components: wall, roof, foundation) are decisive for the storage's capacity, power and efficiency.

Modelling of WGTES during the planning phase represents a challenging step, requiring simplifications of the system. Detailed finite element method/ computational fluid dynamics approaches are not well suited for investigating a variety of possible design scenarios due to excessive computation times. Consequently, there is a high demand for the development and improvement of alternative models for the simulation and performance estimation of WGTES. In our study, we exploit a recently established model "STORE", which depicts a storage within a 2.5-D approach (vertically structured as layers, horizontally structured in predefined directions, cf. abstract figure) and resolves the facility on the building component level. Since "STORE"is characterized by a high level of versatility, it can be used to analyze a range of design scenarios and employed as a planning instrument.

In our presentation, a case study is set up to investigate a variety of technical specifications and to find optimum design solutions: For a given location with climatic and subsurface conditions, we analyze different geometries of artificial storage basins, various insulation material selections, thicknesses, as well as strategies for WGTES charging and discharging. For this, we focus on different technical solutions for indirect energy transfer from and to the basin and on strategies for storage operation. Using the flexibility of "STORE"for evaluation, the component-design simulations are further used to highlight those key factors with the highest impact on the relevant performance indicators. We compare resulting temperature distributions, capacities, charging/discharging power,

and efficiencies of the scenarios. Based on this, we finally deduce recommendations for improved construction and operation of WGTES.

Participation:

In-Person

References:

Bott, C., Ehrenwirth, M., Trinkl, C., Bayer, P. (2022). Component-based modeling of ground-coupled seasonal thermal energy storages. Applied Thermal Engineering, 118810, doi: 10.1016/j.applthermaleng.2022.118810.

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Energy Transition Focused Abstracts:

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MS12 / **677**

Photoporomechanics: Visualizing and quantifying the evolving effective stress in 3D fluid-filled granular media

Authors: Wei Li[1]; Yue Meng[2]; Ruben Juanes[3]

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Granular media constitute the most abundant form of solid matter on Earth and other astronomical objects. When external forces are applied to granular media, the forces are transmitted in the media through a network of contacts—force chains. Understanding the temporal evolution and spatial structure of these force chains constitutes a fundamental goal of granular mechanics. For decades, our understanding of force chains has been derived from 2D experiments, using quasi-2D photoelastic particles with various shapes. Here, we introduce a new experimental technique, which integrates photoporomechanics [Li et al., PR Applied 2021; Meng et al., PR Applied 2022] into tomography, to observe the temporal evolution of 3D force chains under isotropic compression, triaxial shear and rotary shear. Our experimental study visualizes the alignment and intensification of 3D force chains as the external load changes from isotropic to triaxial shear and rotary shear. We also show that the fluctuation of the continuum-scale shear stresses can be pinpointed to the grain-scale buckling and healing of force chains. This work paves the way for understanding the grain-scale underpinning of localized failure of 3D granular media, such as shear banding of concrete structures and stick-slip frictional motion in tectonic and induced earthquakes.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS05 / 678

Pore-scale modelling of Microbially Enhanced Carbon Mineralization

Authors: michele starnoni[1]; Xavier Sanchez-Vila[2]

[1] *Universitat Politecnica de Catalunya*

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Large-scale implementation of geological carbon sequestration is considered as a key strategy to limit anthropogenic warming to 1.5 −2 ℃, as set out in the Paris Agreement. We are interested in a viable alternative represented by injecting CO2 into reactive rock formations, e.g. basalts, to facilitate rapid carbon mineralization, and therefore increase storage security. Our particular interest lies in microbially enhanced carbon mineralization: biological catalysts are utilized to alter reaction rates and further enhance carbon mineralization.
In this talk, we propose a mathematical formulation of the coupled flow and biogeochemical reactive transport problem at the pore-scale. The model is based on optimal decoupling of the reactive transport equations into conservative and kinetic components. We then discuss the construction of a suitable discretization scheme, as well as its integration with the geochemistry package PhreeqPy. We conclude by presenting preliminary model validation results for the geochemical problem of basalt dissolution followed by calcite precipitation.

Participation:

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References:

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Energy Transition Focused Abstracts:

679

Predicting Velocity Field of Porous Rocks using Convolutional Neural Networks

Author: Saeed Shidvash[None]

Co-authors: Mehrdad Vasheghani Farahani [1]; Mohaddeseh Mousavi Nezhad [2]; Saeid Sadeghnejad [3]

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Abstract
Understanding the fluid flow through porous media is essential in different scientific and engineering fields, such as geosciences, petroleum engineering, and subsurface hydrogen or CO2 storage. Predicting velocity fields in pore spaces is exceptionally challenging, which is usually determined by either numerically via solving governing transport equations at the pore scale or visualisation techniques such as particle image velocimetry (PIV).
Artificial intelligence, especially deep learning methods, has recently received significant attention at the pore scale for various applications. This study implements a deep learning approach based on convolutional neural networks (CNNs) to predict fluid velocity in porous media. To achive this, the PIV is utilized first to experimentally obtain the velocity field in a synthetic microfluidic porous chip. The fluid flow is visualized using an inverted microscope and 8-bit grayscale images are taken from the fluid flowing in the porous structure using a high-speed camera. After the image processing, the flow field is determined using defining optimized window size in the iterative PIV plugin in ImageJ. The produced experimental velocity data are then used in the next stage. Several thousand sub-images with a size of 64x64 pixels are extracted from the original velocity fields. We use 80% of the images for training and the rest 20% for testing purposes. A CNN architecture with multiple layers is trained on the flow field images directly provided by the PIV. The network input is the original porous rock images, and the output is the predicted velocity field map. The network is trained with a learning rate in the range of 10-7 to 10-2 using the Adam optimizer. A typical cost function of L-norms is used to compare the similarity between the predicted images and the ground truth. All training was performed on an Nvidia GeForce GTX 1080 Ti GPU with 11 GB RAM. The results show an excellent agreement between the predicted velocity field and the experimental results from PIV.
Keywords:
Convolutional Neural Network, Particle Image Velocimetry, Velocity Fields, Deep learning

Participation:

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References:

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Energy Transition Focused Abstracts:

Poster / 680

A mixed-wet pore network model for electrolyte imbibition in gas diffusion electrodes

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Knowledge of electrolyte distribution inside Gas Diffusion Electrodes (GDE) is a key feature to improve the electrochemical behaviour of these electrodes. In processes like the chlor-alkali-electrolysis, a porous silver electrocatalyst is brought in contact with the liquid electrolyte and the gaseous reactants at the so-called three-phase boundary. To prevent flooding and to alter the wettability of the electrodes, non-wetting polytetrafluoroethylene is added in the manufacturing process. As shown by experimental work 1, the PTFE content has a high impact of the PTFE content on the electrode performance.

Based on FIB/SEM images of the silver electrodes, Direct Numerical Simulations (DNS) inside the pore system have been carried out using Smoothed Particle Hydrodynamics (SPH). This allows us to track the interface movement in a mixed-wettable porous electrode. Fig. 1 shows snapshots of the simulated filling process of a pore system. Hydrophobicity of the electrode significantly changes with consideration of the contact angle due to the electrowetting-effect [2], which had also be seen in experimentally for this GDE [3].

The DNS is computationally too expensive to model larger parts of the electrode while pore network models are computationally far less demanding. Therefore we combined pore network modelling and rigorous hydrodynamic simulations. First, a skeleton from pore space was extracted from the FIB/SEM-images. Then the skeleton is segmented into different parts of the pore systems. Second, characteristic properties like pore diameter and PTFE-Fraction that covers the pore wall are extracted along the connecting paths.

In a mixed-wet system, the entry pressure does not only depend on geometry and **averaged** wettability, but as well on the **locally resolved** wettability degree. In contrast to conventional pore network models, the highest entry pressure can be not determined by the narrowest nor the widest part of the pore system, but on the **most hydrophobic one**. This can be found by DNS or by more simplified models. Using this data as input, the electrolyte imbibition can be modelled by pore network models on representative electrode volumes.

Participation:

In-Person

References:

References:
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[2] F. Mugele and J.-C. Baret, “Electrowetting: from basics to applications,”J. Phys. Condens. Matter, vol. 17, no. 28, pp. R705–R774, Jul. 2005.
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Energy Transition Focused Abstracts:

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MS01 / 681

Impact of hydrogen trapping in underground porous formations on recovery efficiencies during interseasonal storage injection and withdrawal cycles

Author: Katriona Edlmann[1]

Co-authors: Aliakbar Hassanpouryouzband [2]; Niklas Heinemann [3]; Ian Butler [1]; Eike Thaysen [1]

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To meet the global commitments for net zero carbon emissions our energy mix must transition away from fossil fuels. Hydrogen is gaining increasing recognition as a low carbon energy option to support this energy transition, tackling the hard to abate sectors such as decarbonising domestic and industrial heat, power generation and heavy-duty transport. It can also promote increased renewable energy uptake by acting as an energy store to balance supply and demand. For hydrogen to be deployed at the scales required for net zero, we will need access to large-scale geological storage. Depleted porous gas fields provide both the required TWh storage capacity and production rates that can be delivered over many months. Interseasonal hydrogen storage in underground porous formations involves complex displacement and trapping mechanisms that can influence recovery efficiencies over time and as such the economic feasibility of any underground porous formation hydrogen storage operation.

The talk will present the findings from our ongoing research into hydrogen displacement and trapping in porous media during multiple drainage and imbibition cycles, undertaken using x-ray computed micro-CT, micromodels and conventional core flooding experimental equipment. Our results indicate that hydrogen behaves as a non-wetting fluid filling the centre of the pores, with residual brine in the pore corners and throats. During multiple injection and withdrawal cycles we demonstrate that hydrogen trapping occurs via snap-off of hydrogen ganglia. Our work also demonstrates that the magnitude of the trapping depends on flow rate, pore fluid pressure and pore size distribution. This suggests that appropriate site selection and management of hydrogen injection and withdrawal rates can create the opportunity to minimise hydrogen trapping, optimising recovery efficiencies and the economic feasibility of underground porous formation hydrogen storage operations.

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Energy Transition Focused Abstracts:

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Poster / 683

Post-breakthrough finger evolution in unstable growth processes

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Interface between two phases, for instance two fluids as in viscous fingering, often grows in an unstable way. Fingers emerge from growing instability and compete for the available flux. This leads to effective repulsion between the fingers and screening of the shorter ones. While much interest was put into studying such systems before the interface reaches the boundary of the system, very little is known what happens after breakthrough. We show that a striking transition in growth dynamics takes place as the leading finger reaches the boundary of the system. The shorter fingers revive then and grow toward the leading one forming loops. These effects are observed in classical viscous fingering and microfluidic fracture dissolution experiments, but also in discharge patterns and gastrovascular canal system of jellyfish.

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Energy Transition Focused Abstracts:

Poster / 684

Experimental study on effect of cyclic loading on deformation and AE characteristics of sandstone: Relevant for energy storage

Authors: Milad Naderloo[1]; Edgar Hernandez[2]; Kishan Ramesh Kumar[3]; Auke Barnhoorn[4]; Hadi Hajibeygi[3]

[1] *Technical University of Delft*

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With the advent of climate change, a successful transition towards cleaner renewable energy calls for effective storage options. The utilization of underground energy storage (UES), such as depleted porous reservoirs, can help to overcome the balance between the production and demand of renewable energy. All underground energy storages, such as compressed air energy storage and hydrogen storage, are subjected to cyclic loading due to the sequence of production and injection operations. Thus, understanding the geomechanical behavior of porous reservoir rock under cyclic loading is essential to designing and operating underground storages. This study presents results from the 12 triaxial cyclic laboratory experiments performed on the Red Felser sandstone samples with identical porosity and dimensions. In total, eight triangular cycles were applied for each test, and six piezoelectric sensors recorded the acoustic emission (AE) activities during the experiments. The main objective is to explore how cyclic-related parameters (frequency and amplitude of cycles) affect the deformation mechanism and acoustic emission (AE) evolution in elastic and brittle stress regimes. Results regarding mechanical behavior showed that the total axial inelastic deformation increases by increasing the stress regime and amplitude of cycles. However, this parameter reduces by increasing the frequency of cycles. In addition, Young's modulus computed in the loading ramps of the cycles increased significantly from the first cycle to the second cycle for all the tests. For tests in the brittle regime, the larger the amplitude of cycles, the lower the increase in Young's modulus. The AE analysis showed that major events were recorded in the first cycle, and by increasing the number of cycles number of events, the maximum AE and average AE amplitude decreased. Our experimental results highlight that major mechanical changes and AE activities occur during the first cycle, and the stress regime influences the intensity of AE and mechanical changes. These outcomes can be used to study subsidence, fault reactivation, uplift, and other physical phenomena impacting the reservoir's storage capacity, which are influenced by cyclic sandstone deformation.

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In-Person

References:

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685

Pore-scale modeling of PFAS transport in water-unsaturated soils influenced by nonequilibrium mass-transfer processes in thin water films

Author: Sidian Chen[1]

Co-author: Bo Guo [1]

[1] *University of Arizona*

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Per- and polyfluoroalkyl substances (PFAS) are emerging contaminants that have been shown to accumulate at air–water interfaces in water-unsaturated soils. While air–water interfaces can arise from both pendular rings between soil grains and thin water films on soil grain surfaces, the thin-film air–water interfaces account for over 90% of the total air–water interfaces under field-relevant soil water saturations. However, it remains unknown whether all thin-film air–water interfaces are accessible and how potential nonequilibrium mass-transfer processes in thin water films will govern their accessibility and in turn control the transport of PFAS. We have developed a pore-network modeling framework that considers the adsorption of PFAS at air–water water interfaces and the nonequilibrium mass-transfer processes in thin water films. We perform pore-network modeling simulations in a sandy medium to examine the impact of nonequilibrium mass-transfer processes in thin water films on the accessibility of thin-film air–water interfaces and the transport of PFAS in water-unsaturated soils. Our simulations suggest that strong mass-transfer limitations are present in the thin water films and cause early arrival and long tailing in the breakthrough curves, especially at lower water saturations. The new findings highlight the importance of nonequilibrium mass-transfer processes in thin water films for quantifying PFAS transport in vadose zones.

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Energy Transition Focused Abstracts:

MS05 / **686**

In Situ Bioremediation of Selenium and Nitrate for Full Scale Treatment of Mine Waste in the Elk Valley, British Columbia

Authors: Brent Peyton[1]; Lisa Kirk[2]; M. Jim Hendry[3]

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Active in-situ microbial reduction of nitrate and soluble selenate to selenite and elemental selenium (less mobile) was induced by subsurface methanol injections and can stabilize selenium (Se) in mined waste rock. Biogeochemical processes require careful balancing of oxidants (oxygen and nitrate) and reductants (methanol). Pulsed nutrient injection strategies were used in the field in attempts to minimize near-well biofouling. Molecular biology and biological engineering methods have been used

to characterize the microbial ecology and metabolic capacity of waste rock to treat mine-affected water for mining operations in the Elk Valley, located in southern British Columbia, Canada.

Laboratory scale batch and column studies with native microbes demonstrated the capacity to reduce nitrate and Se in saturated waste rock and showed that oxygen and nitrate inhibition of Se reduction was overcome via carbon addition. Biofilm grown on waste rock in saturated aerobic column tests was capable of 50 to 99% nitrate reduction followed by 40 to 95% Se removal; Se was sequestered in the biofilm predominantly in the zero-valent state. Denitrification and Se reduction was most rapid and efficient under suboxic conditions, and as high as 99% removal.

These results were scaled up to a pilot test and ultimately to a full scale in-situ saturated rock fill bioremediation system treating over 20 million L/d. In-situ biofilm coupons were deployed to track the microbial community structure using 16S rRNA gene sequencing. Applying the tools of molecular biology, bioengineering, geochemistry, and principles of microbial ecology to the understanding of biomineralization/bioprecipitation has been effective for management of nitrate and Se in mining settings.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS01 / **687**

A robust and efficient deep-learning-based surrogate model for CO2 storage in deep saline aquifers

Author: Mengjie Zhao[1]

Co-authors: Yuhang Wang [2]; Hadi Hajibeygi [1]; Marc Gerritsma [1]

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CO_2 sequestration and storage in deep saline aquifers is a promising technology for mitigation of the excessive concentration of the greenhouse gas in the atmosphere. The assessment of the CO_2 plume migration depends on the complex multi-physics-based numerical simulation approaches which require prohibitively high computational costs due to the highly non-linear coupled governing equations and multiscale uncertainties of heterogeneous spatial parameter distributions. This study contributes to the development of an end-to-end deep learning workflow that accurately and efficiently predicts the temporal-spatial evolution of the solution CO_2-brine ratio R_S and gas saturation S_g which are two essential tasks for quantification of the amount of trapped CO_2, given input variable of the heterogeneous permeability fields. To this end, a general multitask learning (MTL) framework is developed and applied for learning the dynamic mappings of R_S and S_g simultaneously. The generalization ability of MTL model can be improved by leveraging the information of related tasks with fewer computational expensive labelled datasets. As a novel development, in this work,

the predictions made for multiple tasks from the same permeability realization are not independent, yet they are expected to be consistent. This is due to the fact that the proposed method utilizes the data-driven cross-task consistency constraints which augments the learning of the related tasks. For several test cases, it is shown that MTL models with jointly learning yields more accurate predictions and leads to models with improved generalization for predicting the migration of CO_2 migration. At the same time, the MTL workflow is 10^3 times faster than a high-fidelity physics-based numerical simulator. Therefore, it can serve as a field-scale applicable alternative to conventional simulators for CO_2 storage management. The developments of the work are made on the basis of the publicly-available DARSim research simulator.

Participation:

In-Person

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MS17 / 690

Use of Controlled Fractures in Enhanced Geothermal Systems

Authors: Harun Rashid[1]; Olufemi Olorode[1]

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Enhanced geothermal systems (EGS) are typically tight and naturally fractured like unconventional oil and gas (UOG) reservoirs, so the leading technology being evaluated for their commercial development is also multistage fractured horizontal wells (MFHW). The state-of-the-art approach of thermal recovery from EGS involves injecting cold water into a multiply fractured horizontal/deviated well and producing hot water from a parallel well above the injector, as in the ongoing Utah FORGE project. Considering the negligible control on hydraulic fracture size and orientation, the actual injection and production wells may not intersect planar and bi-wing hydraulic fractures in the ideal and optimum configurations they are simulated. This, coupled with the well-known risk of short-circuiting certain parts of the fracture network, could result in lower heat recovery from the field compared to the simulated MFHW recoveries. To address this problem, we present an alternative technology that employs unique configurations of mechanically cut fractures to recover heat efficiently from all parts of hot rocks in the subsurface. The precise control over these fractures'location, size, orientation, and conductivity facilitates the design of suitable configurations of intersecting fractures.

This paper presents high-resolution numerical studies of thermal recovery from both MFHW and the proposed approach. We simulated several cases with and without stochastic natural fractures

to evaluate the performance of these technologies in such systems. To facilitate a reasonable comparison between the MFHW and the proposed technology, we ensure that the total fracture surface area is the same. The results from the natural stochastic fracture systems studied indicates that the contribution of natural fractures to heat recovery is minimal in the proposed approach. This is due to the flexibility in designing the mechanically cut fractures to avoid being short-circuited by large natural fractures or faults known to be present in the subsurface. We simulated several cases, including one based on the published model parameters of the Utah FORGE project. All these simulation results show that the proposed approach can recover 50% to 140% more thermal energy than the state-of-the-art approach based on MFHW.

The temperature profiles after simulating 50 years of thermal recovery show that the precise control over the location of the fractures allows the reliable and efficient recovery of heat from all parts of the EGS, which could be the key to their commercial development. Finally, the control over the location, size, orientation, and aperture of the mechanically cut fractures provides more reliability in comparing the system modeled to the actual EGS in the subsurface. In contrast, the actual MFHW system could be much less efficient than the simulated system because of the lack of control over the hydraulic fractures' size, orientation, and geometry. There is also no guarantee that the injection and production wells will intersect all the hydraulic fractures.

Participation:

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MS08 / **691**

Dispersive transport dynamics in porous media emerge from local correlations

Authors: Lucas Goehring[1]; Felix Meigel[2]; Thomas Darwent[1]; Leonie Bastin[3]; Karen Alim[4]

[1] *Nottingham Trent University*

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Understanding and controlling transport through complex media is central for a plethora of processes ranging from technical to biological applications. Yet, the effect of micro-scale manipulations on macroscopic transport dynamics still poses conceptual conundrums. Here, we will demonstrate

the predictive power of a conceptual shift in describing complex media by local micro-scale correlations instead of an assembly of uncorrelated minimal units. Specifically, we will show that the nonlinear dependency between microscopic morphological properties and macroscopic transport characteristics in porous media is captured by transport statistics on the level of pore junctions instead of single pores. Probing experimentally and numerically transport through two-dimensional porous media while gradually increasing flow heterogeneity, we find a non-monotonic change in transport efficiency. Using analytic arguments, we built physical intuition on how this non-monotonic dependency emerges from junction statistics. This suggests the value of a shift in perspective towards larger-level structural elements that can broadly affets our understanding of transport within the diversity of complex media.

Participation:

In-Person

References:

Meigel et al., Nature Communications 13:5885 (2022). DOI:10.1038/s41467-022-33485-5

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Energy Transition Focused Abstracts:

MS03 / 692

Developing Methods to Assess Changes in Mechanical Properties of Shale Modified by Engineered Mineral Precipitation

Author: Kayla Bedey[1]

Co-authors: Matthew R. Willett [1]; Laura Dobeck [1]; Joe Eldring [1]; Dustin Crandall [2]; Johnathan Moore [2]; Jonny Rutqvist [3]; Al Cunningham [4]; Adrienne Phillips [1]; Catherine Kirkland [1]

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Fractures in subsurface shale formations serve multiple purposes, for example, in the recovery of resources in hydraulic fracturing or as potential harmful leakage passages through caprocks that may contribute undesired fluids to the atmosphere or functional groundwater aquifers. A proposed method to seal or influence fracture properties is Ureolysis-Induced Calcium Carbonate Precipitation (UICP), a bio-mineralization technology driven by the enzymatic hydrolysis of urea, resulting in the formation of calcium carbonate. Sporosarcina pasteurii is a common microbe used as the source of the urease enzyme that catalyzes the chemical reaction. The resulting calcium carbonate can bridge the gaps in fractured shale and reduce fluid flow through fractures. However, there is little information on how this process affects the mechanical properties of the resulting biomineralized shale. This study represents the first step toward determining the influence of UICP treatment on shale material and its subsequent mechanical strength properties. This methods development study aims

to determine the effect that temperature has on the tensile strength of intact, unfractured shale cores (2.54 cm (1 in) diameter, 5.08 cm (2 in) long). Tensile strength was determined indirectly using a modified Brazilian test where the splitting tensile strength is attained by applying a compressive load onto the core. Shale cores from Eagle Ford and Wolfcamp formations were tested at both room temperature and 60℃ to determine if increased temperature influences the tensile strength of the rock. This data will help to assess the necessity of testing biomineralized cores at temperature. Though 60℃ may not mimic subsurface temperatures of the shales used in this study, it was chosen due to limitations of the UICP process while still approaching temperatures of shale formations. This project aims to evaluate what effect temperature has on the mechanical properties of intact shale cores so that engineered or natural rock fractures that are sealed by biomineralization can be better understood.

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Energy Transition Focused Abstracts:

MS07 / **693**

Multiscale Extended Finite Element Method for the Simulation of Contact –Frictional Behaviors of Fractures Under Compression

Author: Fanxiang Xu[1]

Co-authors: Lambertus J Sluys [1]; Hadi Hajibeygi [1]

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Fractures in the geological formations can propagate and slide when the in-situ compressive stress state changes. As for the compressive nature of the stress, shearing (i.e., Mode II mechanical failure) is the dominant fracture propagation mechanism. In addition, geological formations entail several fractures which can also cross each other. To avoid the use of excessively high-resolution meshes, while resolving the explicit fractures, the extended finite element method (XFEM) is used. The XFEM enriches the FEM continuous space by discontinuous functions so the cracks are explicitly and accurately captured. The linear momentum balance equation is then supplemented by the Mohr-Coulomb friction law, which states the maximum friction a fracture element can tolerate. Additionally, in this work, further constraints are applied to ensure no penetration of elements takes place as a result of significant deformations.

For the simulation of highly fractured geological formations, applying XFEM directly is computationally infeasible, due to the excessive number of extra degrees of freedom (DOFs). To resolve this challenge, we propose this multiscale extended finite element method (MS-XFEM) to simulate the fractures propagation under compressive loading in geological formations. Local XFEM-based basis functions are constructed to capture the compression and the sliding of fine-scale fractures. In each time step when the fractures propagate, the basis functions are updated adaptively in certain

regions where fractures geometries are changed. Using these basis functions, a very efficient FEM-based coarse-scale system is developed since it has no extra DOFs. Once the coarse-scale solution is obtained, it is prolonged to the fine-scale original resolution using the basis functions. This approximate fine-scale solution is then used to estimate the group of growing fractures tips and their growing angles. This allows for exploiting the locality of the propagation process fully while solving a global system. To control the error, an iterative procedure is also developed. MS-XFEM casts a promising method for field-scale applications.

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MS06-B / 694

The Effect of Porous Medium Wettability on the Relationship Between Capillary Pressure, Saturation, and Interfacial Area for Three-Phase Flow

Authors: Dorthe Wildenschild[1]; Rebecca Paustian[1]

[1] *Oregon State University*

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It has become increasingly common to examine multi-phase flow systems in the context of thermodynamics, with the aim of expanding the traditional capillary pressure-saturation (Pc-Sw) relationship to remove its dependence on the history of the system. A commonly used multiphase flow theory based on rational thermodynamics introduces specific interfacial area of fluid-fluid interfaces, anw (interfacial area per unit volume of the porous medium), as a separate thermodynamic entity to extend the Pc-Sw relationship and better describe the the system, including hysteresis. Past pore-network models and 3D imaging experiments have verified that the Pc(Sw, anw) relationship can uniquely describe two-phase flow under quasi-equilibrium conditions, but very limited work has considered three-phase-flow systems, and in particular the issue of interfacial area formation under three-phase-flow conditions for systems of varying wettability.
In this study, we examine the impact of porous medium wettability on three-phase-flow systems. High resolution three-dimensional images, allowing us to measure and analyze capillary pressure, saturation, and interfacial area throughout water and gas invasion (imbibition and drainage scenarios), were generated using x-ray microtomography. The experimental data allows us to evaluate the contact angle behavior for the various fluid pairs under both water-wet and oil-wet conditions, and demonstrated a significant difference in the three-dimensional capillary pressure-saturation-interfacial area relationship as wettability was altered from water-wet to a fractionally-wet.

Participation:

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Energy Transition Focused Abstracts:

Poster / 695

Incorporating Bubble Evolution and Transport in Constitutive Relationships for Quasi- and non-Equilibrium two-Phase Flo

Authors: Douglas Meisenheimer[1]; Dorthe Wildenschild[2]

[1] *Stanford University*

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Bubble generation and transport play a role in many subsurface processes. Production and/or mobilization of gas is for instance observed in biogenic production of methane in peats, and in association with leakage from engineered geologic CO2 storage systems. Other subsurface engineered systems include in-situ air sparging in conjunction with soil vapor extraction, and electrical resistance heating. Thus, there is a need to better understand the presence and transport of bubbles in multi-phase subsurface porous media so that that these processes can be accurately described, and more efficient engineered solutions can be developed.
To this end, constitutive relationships between geometric state variables (fluid curvature, Jnw; nonwetting phase volume, Vn; interfacial area, anw; and Euler characteristic, χ_n) have become increasingly more common in efforts to uniquely predict the state of a two-fluid flow system.
Both lattice Boltzman simulations and fast microtomography experiments have shown that a geometric state function using the non-dimensionalized invariant properties of saturation, specific interfacial area, and Euler characteristic can uniquely predict the mean curvature of the system for both quasi- and non-equilibrium conditions, however, the presence of bubble evolution and transport has not been explored. This study investigates whether the geometric state function remains unique with the inclusion of bubble generation and transport under quasi- and non-equilibrium two-fluid flow.

Participation:

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References:

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Energy Transition Focused Abstracts:

MS17 / 696

Thermal properties of unconsolidated sediments and borehole back fill materials for ground source thermal energy systems

Authors: Cjestmir Hockin[1]; Zanne Korevaar[2]; Jan Diederik van Wees[2]

Co-authors: Stefanie Bus [2]; Ruud Schotting [3]

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The performance of Ground source heat pump systems (GSHP), and heat losses along well bores of high-temperature aquifer thermal energy storage systems (HT-ATES) and geothermal wells is strongly affected by conductive properties[(1,2)].

The anticipated growth of the geothermal and HT-ATES in line with global potential of geothermal energy production of between 125 and 1793 EJ/yr [(3)] augments to the relevance of in-depth understanding of conductive properties. Apart from heat losses affecting performance, shallow groundwater used for drinking water could be affected by the heat transfer[(4,5)]. This can result in (bio)chemical changes in the water composition[(5,6)]. This could potentially reduce the amount of suitable drinking water reserves for future use. In addition, too much heat loss in the cold subsurface could yield a risk of the formation of thermal plumes, which could in turn compromise the production of neighboring geothermal wells in urban areas[(7)].
Uncertainties in the thermal conductivity of an aquifer can affect the efficiency estimations of a single HT-ATES doublet. Using DoubletCalc[(8)], it was determined that this especially plays a role during the initial three loading cycles with a difference of up to 3.5% in efficiency. Others have shown even larger impacts, where an increase of 12.5% of the thermal conductivity reduces the total aquifer technical potential with 25–33%, while decreasing by 12.5% results in a 29–49% increase[(3)].

Understanding and being able to measure and predict the thermal properties both on the centimeter- and meter scale is challenging. Experimental determination is typically on the millimeter scale, most numerical simulations use solid rock-, oil and gas- and construction industry values and well thermal response tests lumpsum many different sediment types into one value.

A semi-automated setup was developed based on the needle-probe method to create an experimentally based understanding of the influence of different interrelated physical properties of unconsolidated sediments on the thermal properties of such sediments. Through a series of experiments, the impact of several sediment configurations have been investigated. Sediments were selected with various amounts of complexity in the composition or layers or layered orientation. For parameter isolation and model calibration, the impact of grain size, shape, porosity and water content was determined using amorphous soda-lime glass.

A numerical model with a radial symmetric finite volume formulation was used to determine the various thermal properties of the sediment sample, using an ensemble smoother with multiple data assimilation (ES-MDA) to inverse fit the model to the experimental data.

The combined experimental-numerical approach provides a reliable and reproducible method for determining the thermal properties of unconsolidated sediments and porous media in general and a means to determine the validity of the numerical model calculations. In oncoming research projects, the experimentally validated results will provide the input for upscaling and validation in a real life ground source heat pump setup.

Participation:

In-Person

References:

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MS21 / **697**

Effect of yield stress in a two phase pore network model

Author: Andreas Hennig[1]

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Non newtonian fluids in porous media flow offers complex interplays that are not fully understood. The Bingham rheology is an approximation of the rheology of a non-Newtonian fluid presenting yield stress, which are useful in several engineering applications, as reinforcement of soils by injection of slurries 1 and in the timely topic of fracking processes [2]. The subject is notoriously hard to study numerically, as we have a nonlinear rheology in a complex porous structure, but there has been recent advances in the field, for instance in characterizing a Darcy law [3]. This work aims to investigate the flow conditions of the Bingham body in complex geometries by using a Pore Network Model with a fairly novel numerical solver in the Augumented Lagrangian Method – a method recently introduced by Talon and Hansen [4]. We are using the model to describe the qualitative behaviors of the yield stress effect, and have characterized a power law behavior that deviates from existing litterature, as found in [3] and [5].

Participation:

In-Person

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Energy Transition Focused Abstracts:

698

Numerical study of hydrodynamic interactions in coupled free-flow and porous media in laminar flow regime

Author: Chakradhar Kakumani[1]

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In this work, we perform numerical computations to study the single-phase hydrodynamic interactions in coupled free-flow and porous media in the laminar flow regime of Reynolds number (Re) in the range 0.1–300. In the porous media, 80×20 micro-size square pillars are arranged in a uniform pattern with a porosity of φ=0.75. Pore-scale simulations are performed in a finite-volume based computational fluid dynamics solver ANSYS Fluent for an incompressible single-phase fluid. We validate our numerical solver with the experimental data of Terzis et al. (2019) for the same geometrical configuration of the porous media at a low Re (=0.14). The primary objective of this study is to investigate how the channel flow interacts with the porous media at various Re and to develop the interfacial boundary condition for the coupled system. The local distribution of velocity components along the interface of the porous media are plotted as a function of Re. From the velocity contours, we observe that the flow enters the porous media at the beginning and leaves the porous media at the end by moving along the streamwise direction at the middle of the porous media. Thus, at the interface, the y-velocity is higher at the beginning and end of the porous medium with opposite flow directions, but in the middle, it is almost negligible. Therefore, a U-shaped velocity profile is observed in the porous domain. Flow recirculation zones are also observed in the porous media when Re≥50, which gradually vanishes towards the bottom and the middle of the porous zone. The streamwise velocity is plotted along the y-direction at the beginning, the middle, and the end of the porous zone. The x-velocity component is significantly higher in the free-flow channel and drastically drops in the porous medium. Owing to the presence of no-slip micro-pillars, the velocity fluctuates sinusoidally along the vertical location. Pore-scale simulations show that parallel flow does not exist at the interface of the porous and channel flow. The fluid periodically crosses the interface, creating small-scale U-shaped flow profiles between the pores of first row of pillars. The volume averaged velocity shows a slip condition at the interface (y=0). The effect of Re on the flow field is only noticed at a region closed to the interface, while the effect of Re is negligible in other parts of the domain. Thus, the interfacial velocity-slip is evaluated based on the Beavers-Joseph model by volume-averaging of the numerical data at different Re. The Beavers-Joseph coefficient changes along the interface and decreases as the flow deviates from the Poiseuille flow. With increase in Re, we observe an increasing trend in average values of the Beavers-Joseph coefficient. This work finds applications in various multi-scale natural and industrial processes, which include atmospheric flows, transpiration cooling, convective drying, water management in fuel cells, metal foam heat sinks for electronics cooling, and aerospace compact heat exchangers embedded with porous materials.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

MS13 / 700

Flow enhancement in nano-channels using surface acoustic waves

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Flow through micro-nano channels is ubiquitous in nature, such as flow inside biological nanoporins in all living beings, vascular motion in fungi, and intestinal flow due to contractions of walls. It is also present in a vast range of engineering and biomedical applications like nanorobotics, printing technology, quantum computing, optics, chemical process control, drug delivery, and cell biology. Due to the high surface-to-volume ratio, energy dissipation inside the micro/nano channel is significantly large. As a result, flow inside micro/nano channels is extremely inefficient compared to macroscale channels. Traditional approaches to enhance flow inside micro/nano channels involve making the channel wall hydrophobic 1 or changing the surface morphology [2] to reduce friction. Xie and Cao [3] showed that the flow rate inside nanochannels could be enhanced by reducing channel wall friction with the application of traveling surface waves. However, the frequency of the applied surface wave was extremely high (in THz order) in their work, which is difficult to obtain with state-of-the-art surface acoustic devices. Marbach et al. [4], using mathematical formalism, revealed that wiggling of the nanochannel wall due to thermal fluctuations could significantly enhance diffusion and, therefore, increase the flow rate. They also showed that active surface wiggling produced by external stimuli could also augment the flow rate. However, the detailed understanding of this flow enhancement is still far from satisfactory. Therefore, we perform Molecular Dynamics simulations to analyze the acoustic wave-driven flow behavior inside nanochannels at the molecular scale. Contrary to the previous work, we observe a reduction in the flow rate at low frequencies of vibration; the flow rate starts increasing beyond a certain frequency. The decline in the flow rate is attributed to the hindrance to the flow produced by the "roughness"of the surface during the propagation of the surface wave. Our results show that the magnitude of the local velocity across the channel increases significantly; however, the velocity profile remains parabolic —the profile doesn' t widen and flatten with higher frequencies. This is indicative of the fact that the flow enhancement is not only due to the reduced friction at the wall but also due to increased bulk fluid motion due to the acoustic pressure produced as a result of traveling surface waves. Our study also reveals that the nanochannels with a hydrophobic surface produce better flow enhancement in response to traveling surface waves. Our work provides insights to better design strategies for surface acoustic wave-driven flow enhancement inside nanochannels.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / 701

Identification and understanding of colloidal destabilization mechanisms in geothermal processes

Authors: Ines Raies [1]; Marc Fleury[1]; Eric Kohler [1]; Béatrice Ledésert[2]

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In this work, the impact of clay minerals on formation damage of sandstone reservoirs is studied to provide a better understanding of the problem of deep geothermal reservoir permeability reduction due to fine particle dispersion and migration. In some situations, despite the presence of filters in the geothermal loop at the surface, particles smaller than the filter size (<1 µm) may surprisingly generate significant permeability reduction affecting in the long term the overall performance of the geothermal system.
Our study is carried out on cores from a Triassic reservoir in the Paris Basin (Feigneux, 60 km Northeast of Paris). Our goal being to first identify the clays responsible for clogging, a mineralogical characterization of these natural samples was carried out by coupling X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS). The results show that the studied stratigraphic interval contains mostly illite and chlorite particles. Moreover, the spatial arrangement of the clays in the rocks as well as the morphology and size of the particles suggest that illite is more easily mobilized than chlorite by the flow in the pore network.
Thus, based on these results, illite particles were prepared and used in core flooding in order to better understand the factors leading to the aggregation and deposition of this type of clay particles in geothermal reservoirs under various physicochemical and hydrodynamic conditions. First, the stability of illite suspensions under geothermal conditions has been investigated using different characterization techniques including Dynamic Light Scattering (DLS) and Scanning Transmission Electron Microscopy (STEM). Various parameters such as the hydrodynamic radius (around 100 nm), the morphology and surface area of aggregates were measured.
Then, core-flooding experiments were carried out using sand columns to mimic the permeability decline due to the injection of illite-containing fluids in sandstone reservoirs. In particular, the effects of ionic strength, temperature, particle concentration and flowrate of the injected fluid were investigated. When the ionic strength increases, a permeability decline of more than a factor of 2 could be observed for pore velocities representative of in-situ conditions. Further details of the retention of particles in the columns were obtained from Magnetic Resonance Imaging and X-ray Tomography techniques, showing that the particle deposition is non uniform along the column.
It is clearly shown that very fine particles as small as 100 nm can generate significant permeability reduction under specific conditions in high permeability porous media representative of the Triassic reservoirs of the Paris basin. These retention mechanisms are explained in the general framework of the DLVO theory.

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Poster / 702

Pore-scale hysteresis and Relative Permeabilities in Edwards Brown Dolomite

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Carbon dioxide storage in subsurface formations is a promising technology for mitigating climate change, but a good understanding of the flow behaviour in targeted reservoirs is crucial. Heterogeneities at various scales can significantly impact flow behaviour, especially in carbonate reservoirs, which contain a large portion of the world's hydrocarbon reserves. In this study, we used an experimental method to examine hysteresis, heterogeneity, and relative permeabilities in multiphase flow in Edwards Brown dolomite. The experiment was conducted on a water-wet sample using brine (20% KI) and oil (decane) at a resolution of 5.6 μm during steady-state drainage and imbibition cycles. Our goal is to describe the effect of heterogeneities on the fluid behaviour, saturation changes, and residual trapping to improve the upscaling from the pore scale to the core scale to better represent the underlying pore-scale processes at the Darcy scale in a consistent way.

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MS01 / 703

CT visualization of the CO2 degassing process in porous media

Authors: Chris Boeije[1]; Cas Verweij[1]; Anushka Tripathi[1]; Pacelli Zitha[2]; Anne Pluymakers[1]

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Geothermal fluids tend to contain large quantities of dissolved gasses such as CO2 and N2. A drop in pressure towards the production well means that free gas bubbles can form as the solubility limits can be exceeded. These bubbles occupy part of the pore space thereby leading to a decrease of the water relative permeability, thus leading to reduced production of geothermal waters. In addition, the presence of free CO2 can enhance the rates of precipitation of minerals such as calcite (Stefánsson et al., 2016).
This project is aimed at experimentally investigating the conditions at which the onset of the degassing process starts (i.e. the conditions where the first free gas bubble forms) inside porous media. In addition, the influence of presence of free gas bubbles on the water relative permeability of the porous medium is assessed.
A series of coreflood experiments was carried out where CO2 along with an aqueous phase (either tap water, 1 M NaCl brine or 1.5 M CaCl2 + 2 M NaCl brine) were co-injected into a Berea sandstone core at ambient temperature. The CO2 concentration ranged from 0.2 to 1.3 mol/L to assess its influence on the degassing pressure. Initial coreflood tests outside the CT scanner using a vertically oriented core showed an abrupt decrease in the water relative permeability of approximately 90% at pressures just slightly below the degassing pressure. This implies that the free gas bubbles function as an effective blocking agent in these rocks thus limiting the water production rate. The onset of degassing (i.e. pressure below which degassing is observed) is also found to correlate well with CO2 solubility values that were obtained using the Van ʻt Hoff equation (Smith and Harvey, 2007) when using tapwater as the aqueous phase, but with larger deviations found at higher brine salinities.
The first series of CT assisted corefloods was performed using a medical CT scanner and the same experimental conditions as the earlier experiments. Here the core had to be placed horizontally due to limitations of the scanner. Free gas saturations within the core were determined at various different back pressure levels and compared with differential pressure logs. Again, an abrupt transition in the water relative permeability was found once degassing started, but the process also suffered from gravity override of the free gas especially at higher CO2 concentrations.
Additional coreflood experiments are currently being prepared utilizing a new CT scanner that allows for vertical placement of the rock core along with higher resolution scans. This enables performing tests without gravity override problems. Also, the higher resolution scans allows capturing of more details of the degassing process, such as mineral precipitation.

Participation:

In-Person

References:

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MS08 / 704

Chaotic mixing due to oscillatory flow in porous media

Authors: Gaute Linga[1]; Tanguy Le Borgne[2]

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Solute mixing in time-periodic porous media flows is relevant to a wide range of natural, industrial and biological processes spanning from seismicity through hydropeaking to pulsatile flows in biological tissue. Nevertheless, it remains poorly understood how the (spatial) frequencies of the porous medium and the (temporal) frequencies of the time-varying flow field interplay and affect the mixing dynamics. Here we investigate the dynamics of solute mixing by a single-frequency oscillatory flow through an archetypal porous medium consisting of periodically arranged cylindrical obstacles. By extensive high-resolution pore-scale simulations, we find that successive stretching and folding events across stagnation points generate chaotic mixing, meaning that fluid elements are elongated exponentially in time. We propose a theoretical model allowing us to analytically predict the Lyapunov exponent based on the frequency and amplitude of the flow. The model opens new avenues for predicting mixing and reaction rates across a host of time-dependent porous media flows.

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Energy Transition Focused Abstracts:

MS10 / 705

Use of 4D tomography to track the evolving geometry and flow patterns in dissolving rocks

Authors: Piotr Szymczak[1]; Max P. Cooper[1]; Rishabh P. Sharma[1]; Andrzej Radliński[2]; Tomasz P. Blach[2]; Katarzyna Drabik[3]; Alessandro Tengattini[4]

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Dissolution of porous media introduces positive feedback between fluid transport and chemical reactions at mineral surfaces leading to the formation of pronounced wormhole-like channels. While the impact of flow rate and reaction rate on the shapes of the wormholes is now well understood, much less is known about the dynamics of their propagation. In this communication, we show how the evolution of wormholes and their effects on flow patterns can be captured by in-situ X-ray microCT imaging of dissolving limestone cores. 4D tomography allows us in particular to correlate the permeability changes in a dissolving core with the advancement of the tip position of the wormhole. The analysis of such correlations allows one to detect the highly cemented regions in the core which

act as permeability barriers, which the wormhole tries to bypass.
Finally, we show how to supplement this information with the analysis of the flow patterns. The latter can be obtained by injecting a contrast solution while scanning the sample in the tomograph. This data allows us to quantify the competition between the wormhole branches, which drives the evolution of the wormholing pattern.

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Energy Transition Focused Abstracts:

Poster / 706

Is mixing chaotic in laminar flows through rocks?

Authors: Alexandre Puyguiraud[1]; Tanguy Le Borgne[2]; Joris Heyman[3]

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Recent studies have shown that chaotic advection is spontaneously produced by laminar flows through granular media such as bead packs, strongly impacting solute mixing rates. This has strong implications for many reactive and biological processes in the subsurface. Chaotic dynamics could also be key in a wide range of environmental and industrial applications driven by mixing. Beside granular media, there is still no evidence that chaos broadly arises in the large variety of porous architectures that exist. In particular, it is unknown how the pore structure and topology can control chaotic dynamics.
In this study, we numerically investigate the mixing behavior of solute for a wide range of natural and engineered porous material that goes from carbonates and sandstones to beadpacks. We quantify chaotic advection by measuring Lagrangian stretching statistics (Lyapunov exponent) and its impact on mixing by estimating the decay of solute concentration variance. We find that stretching and mixing rates vary significantly between the different classes of porous architectures. We also observe that the flow resolution can dramatically impact the statistics and give guidelines for an accurate computation of the Lyapunov exponent.

Participation:

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MS03 / **708**

Multipoint mixed FEM for rotation-based poroelasticity with faults

Author: Alessio Fumagalli[1]

Co-authors: Wietse Boon [1]; Anna Scotti [1]

[1] *Politecnico di Milano*

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In this work, we present a mixed finite element formulation of the Biot problem based on the rotation and displacement for the elasticity, and Darcy velocity and pressure, for the fluid phase flow. The discretization of the problem is based on exact discrete complexes and also on a suitable choice of a quadrature rule to localize, in a multi-point fashion, and thus algebraically eliminate the rotation and flux variables. The resulting method has fewer degrees of freedom than the original one, leading to a cost-effective formulation of the poroelastic problem with a two fields formulation. Indeed, we consider lowest order Raviart-Thomas finite elements for the displacement and piece-wise constants for the fluid pressure, thus the number of degrees of freedom is equivalent to a mixed formulation of a single-phase flow. Numerical results show the expected convergence rates for the errors for all the variables, for both the four and two fields formulations. We extend this discretization strategy to account for faults, which are three-dimensional physical objects where one of the dimension (their thickness) is orders of magnitude smaller than the others, and their material properties might be very different than the surrounding porous media. To avoid excessive mesh refinement, in the discrete setting, we represent them as objects of codimension one and consider a new set of equations based on a dimensional reduction strategy. We can thus reformulate the problem as mixed-dimensional and exploit the properties of the discrete approximation to obtain reliable solutions at an affordable computational cost. The reference paper for this contribution is 1, see also references therein.

Participation:

In-Person

References:

1 arXiv:2212.12448 [math.NA]

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MS08 / **709**

Computing Fick diffusion coefficients using equilibrium molecular dynamics for binary mixtures of hydrogen relevant for underground hydrogen storage

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Scaling up renewable energy production needs to be accompanied by a concomitant scaling of storage technologies. In this regard, hydrogen (H₂) is an attractive energy carrier due to its large specific energy capacity and its clean combustion products. However, its low mass density requires gigantic volumes (billion m³) to store energy in the order of TWh. Geological formations such as depleted gas reservoirs conveniently provide these large volumes. To maintain a safe operational pressure range, a cushion gas is introduced into the reservoir, which expands and compresses during the storage cycles of H₂. A large compressibility of this gas maximizes the storage capacity of H₂ during injection, and minimal mixing facilitates an efficient recovery of pure H₂ during production. Among many options such as nitrogen, methane and H₂ itself, carbon dioxide is also considered a suitable cushion gas due to its large compressibility at supercritical conditions¹.

On timescales relevant to storage (weeks to years), the cushion gas will mix with H₂ through molecular diffusion and flow-induced mechanical dispersion. This work focuses on molecular diffusion, as the first step towards quantifying mixing of the stored H₂ and the cushion gas. According to Fick's law, the diffusing mass flux is a product of gradient in mole-fraction and the (molecular) diffusion coefficient D. Fick diffusion coefficients exhibit strong dependencies on thermodynamic variables such as the mixture composition, temperature T, and pressure P. In this work, we compute D at various mixture compositions using equilibrium molecular dynamics^[2] for $P \in [20,300]$ bar and $T \in [250,350]$ K for various binary gas mixtures. The analytic expression for diffusion coefficients based on kinetic theory of gases deviates significantly from our predictions - thus emphasizing the need to account for molecular interactions. Furthermore, we provide fit functions to enable fast and accurate prediction of diffusion coefficients at reservoir conditions, which are beneficial for reservoir flow simulators. Finally, the phase equilibria of these gas mixtures are also predicted using molecular simulations.

Participation:

In-Person

References:

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[2] Seyed Hossein Jamali, Ludger Wolff, Tim M. Becker, Mariëtte de Groen, Mahinder Ramdin, Remco Hartkamp, André Bardow, Thijs J. H. Vlugt, and Othonas A. Moultos, Journal of Chemical Information and Modeling 2019 59 (4), 1290-1294

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Energy Transition Focused Abstracts:

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Poster / 710

Investigation of species transport in fractured porous media using 3D-printed micromodels

Author: Alexandros Patsoukis Dimou[1]

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Understanding flow and transport through fractured porous media is vital for optimising large-scale hydrological and geological processes such as carbon capture and storage, geothermal energy production, and contaminant transport. Direct Numerical Simulations (DNS) solving the Navier-Stokes equations can accurately describe species transport through relatively small volumes of porous media. However, the use of DNS to investigate large geometries with multiscale features, such as fractures, pores and micro-pores, is limited due to the significant computational costs. An alternative can be offered by the Multiscale Darcy-Brinkman-Stokes (DBS) simulations, for which under-resolved small-scale features are represented through their effective permeability and porosity values. Multiscale DBS models have been extensively benchmarked for single-phase flow through multiscale porous media. However, relatively little knowledge exists of their applicability to model species transport. Recent advances in three-dimensional (3D) printing allow for fast and cheap manufacturing of multiscale models with complex porosity distributions, which has enabled the investigation of specific flow processes. In this work, we present an experimental and numerical study of species transport through 3D-printed geometries containing both fracture and matrix. First, we conduct single-phase flow species transport experiments in order to develop a benchmark experimental dataset. Then, we compare the experimental results with the species transport obtained with DNS simulations and with multiscale DBS simulations. Our results show an accurate match between the DNS and DBS solvers. Moreover, we show that our multiscale DBS model can be used to extract the transfer function for flow and species transport at the interface between fracture and matrix, which can be used as an input for dual continuum models. Finally, we show how our model can be applied to estimate the transfer coefficients as a function of flow rate and species diffusion using a micro-CT image of a real fracture.

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MS11 / 711

The permeability of pillar arrays in microfluidic devices: an application of Brinkman's theory towards wall friction

Author: Thejas Hulikal Chakrapani[1]

Co-authors: Hanieh Bazyar [2]; Rob Lammertink [3]; Stefan Luding [3]; Wouter den Otter [3]

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Darcy's law describes the flow of Newtonian fluids through bulk porous media as the product of the applied pressure difference, the fluid's viscosity and the medium's permeability. Brinkman extended Darcy's law with a viscous stress term, thereby enabling boundary conditions to the flow field at the surface of the medium. The validity of Brinkman's term, and the value of its effective viscosity, have been heavily debated since their introduction nearly 75 years ago. We use experiments and Multibody Dissipative Particle Dynamics (MDPD) simulations to study flows through ordered and disordered pillar arrays in microfluidic channels of limited height. We find that the simulated velocity profiles are well described by an expedient interpretation of Brinkman's theory. Depending on the solid volume fraction and pillar arrangement, the effective viscosity varies between two and three times the bulk fluid viscosity. The calculated effective permeabilities of the flow devices, combining the flow resistances due to the pillars and the walls by Brinkman's theory, agree well with the experimental data. This approach enables fast and accurate estimates of the effective permeability of micropillared chips. The simulated force distributions over the walls and pillars require an effective viscosity equal to the bulk viscosity and an elevation-dependent permeability of the pillar array.

Participation:

In-Person

References:

The permeability of pillar arrays in microfluidic devices: an application of Brinkman's theory towards wall friction,
Thejas Hulikal Chakrapani, Hanieh Bazyar, Rob Lammertink, Stefan Luding, Wouter K. den Otter, Soft Matter, 2023, DOI: 10.1039/d2sm01261h

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Energy Transition Focused Abstracts:

712

Analysis of the potential of CO2 Sequestration in the Washita-Fredericksburg Formation

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Sedimentary rock deposits in the southeast of the United States are known to be adequate reservoirs for carbon sequestration. One of these formations is the Washita-Fredericksburg formation in southwest Alabama. Although studies have suggested that this Cretaceous sedimentary formation could act as a great CO2 reservoir, there is not much known about this formation. In this study, sandstone samples of the Washita-Fredericksburg formation were analyzed to (1) understand their mineralogical composition and porosity and (2) to understand potential geochemical processes that might occur in the formation between CO2 and the sandstones. XRD and SEM data showed that the sandstone samples are mainly composed of quartz, k-feldspar, albite, and clay minerals such as smectite and kaolinite. Mineral dissolution rates were obtained from previous studies at different temperatures, and the final value was calculated using the formation temperature (68° C) at a sample depth (2.6 km). Mineral surface areas were obtained from low, high, and average BET surface areas given by previous studies. CrunchFlow was used to calculate brine composition and initial pH in the formation. After obtaining all the necessary data, a reactive transport model was built in Crunchflow. The results in this model show possible geochemical changes in porosity, mineral volume percentages, and ion concentrations. The results from this model gave more insight and a better understanding of potential changes in porosity and permeability in porous CO2 reservoirs. Understanding the effects of CO2 and porous media is crucial since there can be changes in porosity, permeability, and possible mineral precipitation. These changes can affect formation properties. This project is supported by the Southeast Regional CO2 Utilization and Storage Partnership (SECARB-USA), funded by the U.S. Department of Energy.

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Energy Transition Focused Abstracts:

MS09 / 713

Steady-state flow transitions in ordered porous media investigated using an artificial compressibility finite difference method

Author: Tobias Forslund[None]

Co-authors: Staffan Lundström [1]; Sofia Larsson ; Gunnar Hellström [2]

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Steady-state transitions in porous media, here defined as a discontinuity in one or more macroscopic observables as a function of Reynolds number while the flow remains steady, are known to occur for a multitude of different types of porous media. In previous studies, it has been discovered that these transitions coincide with the development of inertial cores and a reduction in the spatial variance of the velocity field 1. Recently, flow through an ordered porous media cell consisting of a staggered cylinder packing was investigated using tomographic particle image velocimetry [2]. The results reveal a complex three-dimensional steady-state flow pattern, occurring in the region where inertial effects are expected to become dominant. The peculiar flow pattern, which significantly increases the vorticity and flow resistance, indicates that the transition may need more explanation than the development of inertial cores as suggested by earlier studies.

The investigation is confined to single-phase, fully saturated Newtonian flow through porous media. By making use of an in-house GPU implementation of an artificial compressibility finite difference method the transition from the stokes flow region, to the end of the steady inertial region, is performed on three types of ordered porous media. These are a staggered packing of mono-radii cylinders, a staggered packing of quadratic cross-section rods and a body-centred cubic packing of mono-radii spheres as disclosed in the figure. Here, also the flow regions are presented where the Reynolds number increases from left to right and the velocity magnitude is visualized by a volume rendering. When increasing the Reynolds number it is concluded that in addition to the transition resulting in an increase of the spatial variance of the velocity, as known from earlier studies, it coincides with a rise in the absolute value of the pressure integral across the solid surfaces. These observations, together with an observed increase in the absolute value of the pressure velocity coupling, indicate that the flow tends to alternative flow paths which reduces impingement on the solid surfaces.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS07 / 714

Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions

Authors: Markus Knodel[1]; Serge Kräutle[2]; Peter Knabner[2]

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In order to study the efficiency of the various forms of trapping including mineral trapping scenarios for CO_2 storage behavior in deep layers of porous media, highly non-linear coupled diffusion-advection-reaction partial differential equations (PDEs) including kinetic and equilibrium reactions modeling the miscible multiphase multicomponent flow have to be solved. We apply the globally fully implicit PDE reduction method (PRM) developed 2007 by Kräutle and Knabner for one-phase flow, which was extended 2019 to the case of two-phase flow with a pure gas in the study of Brunner and Knabner. We extend the method to the case of an arbitrary number of gases in gaseous phase, because CO_2 is not the only gas that threats the climate, and usually is accompanied by other climate killing gases. The application of the PRM leads to an equation system consisting of PDEs, ordinary differential equations, and algebraic equations. The Finite Element discretized / Finite Volume stabilized equations are separated into a local and a global system but nevertheless coupled by the resolution function and evaluated with the aid of a nested Newton solver, so our solver is fully global implicit. For the phase disappearance, we use persistent variables which lead to a semismooth formulation that is solved with a semismooth Newton method. We present scenarios of the injection of a mixture of various gases into deep layers, we investigate phase change effects in the context of various gases, and study the mineral trapping effects of the storage technique. The technical framework also applies to other fields such as nuclear waste storage or oil recovery.

Participation:

In-Person

References:

Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions. Comput Geosci 26, 697-724 (2022). M.M. Knodel, S. Kräutle, and P. Knabner. doi.org/10.1007/s10596-022-10140-y

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716

Experimental and triple-layer surface complexation modelling study: influence of temperature on interface properties in crude oil-brine system

Author: Yogarajah Elakneswaran[None]

Co-authors: Xingjuan Hao [1]; Dong Kyu Cha [2]; Moataz Abu-Al-Saud [2]; Ayirala Subhash [3]

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The rock wettability influences the distribution of fluids within the pores, which significantly affects oil displacement and recovery efficiency. It has been suggested that the wettability alteration from oil-wet to water-wet improves the oil recovery during the injection of low salinity or smart waterflooding for enhanced oil recovery (EOR). The electrical surface charge, the main interface property, developed at crude oil/brine and rock/brine interfaces affects the wettability alteration. The surface charge is closely related to the zeta potential which can be measured by experiments. On the other hand, the surface complexation models have been used to theoretically interpret the crude oil/brine and rock/brine interfaces and provides insight into the interaction at the crude oil-brine-rock interface. The interface properties strongly depend on pH, brine composition, and temperature. However, only a few studies have reported the effect of temperature on the interface properties.

The main objective of this study is to investigate the effect of temperature on crude oil/brine interface properties. Three crude oils with different total acid number (TAN) and total base number (TBN) were selected for this study. The zeta potential of the crude oil emulsion in the de-ionzed water, high salinity water, low salinity smart water, low salinity CaCl2 solution, and low salinity Na2SO4 brine was measured at 25 ˚C, 40 ˚C, and 60 ˚C. The pH of the selected solution was adjusted from 2.5 to 7.6.

With increasing pH of the solution, the surface of crude oil showed more negative zeta potential due to de-protonation of carboxyl groups in the crude oil. The presence of divalent cations such as calcium or magnesium in high salinity water, smart water and CaCl2 solution compensates the negative surface of crude oil and reduces the absolute value of zeta potential. Overall, the temperature rise in the solution decreases the absolute value of zeta potential. A part of experimental data was fitted to the triple-layer surface complexation modelling results to determine the associated equilibrium constants for the carboxyl group surface reactions. The other part of experimental data was used for the validation of the triple-layer surface complexation parameters. Moreover, the enthalpy changes for the surface complexation reactions of protonation, de-protonation and adsorption of cations were determined from the relationship between temperature and the equilibrium constants, which can be used to estimate interface properties of crude oil-brine system at reservoir conditions.

Participation:

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Energy Transition Focused Abstracts:

Poster / 717

Intracellular ”in silico microscopes” - fully 3D spatial Hepatitis C virus replication model simulations

Authors: Markus Knodel[1]; Arne Naegel[2]; Eva Herrmann[3]; Gabriel Wittum[4]

[1] *Simulation in Technology TechSim*

[2] *Goethe-University Frankfurt*

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[4] *AMCS, KAUST, CEMSE, MaS, Thuwal, Saudi Arabia*

Corresponding Authors: markus.m.knodel@gmx.de, herrmann@med.uni-frankfurt.de, wittum@techsim.org, naegel@gcsc.uni-frankfurt.de

Virus pandemics and endemics cause enormous pain and economic, political, and social costs and turmoil. While the Covid19 pandemics induced obvious damages, the "silent" Hepatitis C virus (HCV) infection induced liver destruction is the main reason for liver transplants. HCV virus replication sometimes serves as some sort of representative to study virus replication basics. HCV-generated virus genome replication factories are housed within virus-induced intracellular structures termed membranous webs (MW) which are derived from the Endoplasmatic Reticulum (ER). The ER is an interconnected intracellular membrane network and embedded within the cytosol. The interplay of virus components whose action is restricted to the 2D ER manifold and of other virus components which act in the 3D volume cytosol space is crucial for virus replication. Up to now, the very advanced experimental data such as highly spatially resolved fluorescence and electro-tomography data in many cases do not enter computational HCV viral RNA (vRNA) cycle models. Based upon diffusion-reaction partial differential equations (PDEs), we are developing fully 3D resolved "in silico microscopes"to mirror in vitro / in vivo experiments for the intracellular vRNA cycle dynamics. Our first models described the major components (vRNA, non-structural viral proteins - NSPs - and a host factor). The next steps incorporated additional parameters: Different aggregate states of vRNA and NSPs, and population dynamics inspired diffusion and reaction coefficients instead of multilinear ones. Our work in progress framework presently is merging effects restricted to the ER surface (e.g. NSP diffusion) with others taking place in the cytosol (e.g. host factor supply). Further we estimate and incorporate realistic parameters such as NSP diffusion constants. The simulations are performed upon experimental data based reconstructed cell geometries which indeed display a very complex porous medium structure. Our simulations help understanding the relation of form and function of intracellular virus replication mechanisms. In the long run, our framework might help to facilitate the systematic development of efficient direct antiviral agents and vaccines.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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Multicomponent bubble ripening in porous media: the case of hydrogen storage

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Bubble trapping in porous microstructures occurs in many applications, such as CO_2 sequestration, underground H_2 storage, and fuel cells. In hydrogen storage, the occupying bubbles are gaseous and vary in composition (due to the presence of cushion gas) and size (or interfacial curvature), resulting in an initial condition that is far from global equilibrium. Since bubbles are partially miscible, they dissolve and diffuse through the wetting phase, thereby exchanging mass with one another. This process is known as Oswald ripening. Prior work on ripening has focused mainly on single-component and incompressible bubbles. Here we present a mathematical formulation of a pore network model that simulates the evolution of thousands of multi-component bubbles in arbitrary microstructures. We show that physics leads to non-trivial and unexpected evolution dynamics not observed in single-component systems. The implications of these observations on the viability and performance of underground hydrogen storage are discussed.

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Energy Transition Focused Abstracts:

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Effect of chemical fluid-solid interaction on physical properties of rocks: a 3D numerical study

Authors: Vadim Lisitsa[1]; Tatiana Khachkova[None]; Yaroslav Bazaikin[1]; Dmitry Prokhorov[1]

[1] *Institute of Mathematics SB RAS*

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We present numerical simulations of CO_2 sequestration in carbonate rocks. Injection of CO_2 leads to partial dissolution of the rock matrix, changing the geometry and topology of the pore space. As a result, the permeability, formation factor, and elastic properties of the rocks also evolve. To characterize the changes in the pore space topology, we used persistent homology methods. We varied the input conditions (flow rate, reaction rate, and diffusion), simulated the reactive transport, and then constructed the persistent diagrams for Betti One numbers (corresponding to closed cycles in the pore space). After that, we introduced the measure in the persistent diagram space and performed clustering with respect to this measure. Four different clusters representing different dissolution

scenarios were stably recovered. Visually, the clusters correspond to slow dissolution, wormholes forming, homogeneous dissolution of the rock matrix, and the formation of the dissolution front. We compared the changes in porosity, absolute permeability, formation factor, and elastic properties of the rocks for different clusters, illustrating that different dissolution scenarios lead to different cross-parameter relations. In particular for the wormholes' formation, small changes in the porosity cause a strong increase in the permeability, whereas softening of the material is relatively low. For the homogeneous dissolution, permeability is less sensitive to the porosity changes, however, the elastic parameters got much smaller.

The research was supported by the RSCF grant no. 21-71-20003

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Energy Transition Focused Abstracts:

MS06-B / 721

Modeling interfaces explicitly with an embedded-boundary finite-volume method across applications

Authors: Sergi Molins[1]; David Trebotich[None]; Carl Steefel [1]

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Porous media are characterized by their physical and chemical heterogeneity at a range of length scales. As a result, the interfaces between the different phases or materials present in the media are complex. Processes near or at these interfaces often exert a controlling effect on the outcome of applications in which these porous media are used. Process-based modeling is a powerful tool to understand how the different processes interact to produce the observed behavior. However, representation of these interfaces in models in order to capture the relevant processes explicitly remains a challenge.

In this presentation, we describe an embedded-boundary method that enables us to incorporate interfaces explicitly in a block-structured finite-volume model. In this approach, the irregular domain created by complex interfaces is discretized as a collection of control volumes formed by the intersection of the problem domain with the cubic Cartesian grid cells, as in a "cut cell"approach. The various operators are approximated by applying the divergence theorem on the irregular control volumes, with the fluxes computed by using primary discretized dependent variables that approximate the solution evaluated at the centers of the original Cartesian cells. Away from the boundary, the finite-volume method reduces to a standard finite-difference approximation.

We demonstrate the approach in three applications to reactive transport in porous media. In all cases, we consider fluid flow, solute transport, aqueous complexation and mineral dissolution-precipitation reactions. The applications cover a range of conceptual models. We start with an application where

the interfaces separate fluid and solid phases and reaction rates are limited by solute transport to the interfaces. We follow with fractured media, where interfaces separate the fracture opening from the surrounding matrix. In this case, transport limitations exist both in the fracture as well as in the matrix. We end with an application to reverse osmosis where the interface acts as a permeable boundary to water but not to ions in solution.

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Energy Transition Focused Abstracts:

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Understanding the impact of small-scale topographies on multi-component reactive transport processes within the groundwater and surface water mixing zone using a fully-coupled modeling framework

Author: Pei Li[1]

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Small-scale riverbed topographies (e.g., ripples) control the extent of groundwater and surface water exchange flux and the resulting biogeochemical processes. There is a lack of understanding on how small-scale topographies impact biogeochemical dynamics such as the aerobic respiration and coupled nitrification-denitrification reactions. Here we present a fully-coupled numerical modeling framework in in OpenFoam that we used to systematically study and understand the controlling influence of 3D and small-scale topographies on the biogeochemical dynamics within the groundwater and surface water mixing zone. Our preliminary results show that the out-of-phase riverbed parameter control and enhance biogeochemical reactions. We also present how the zones of enhanced reaction rates (i.e., hot spots) develop within different riverbed topographies.

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Energy Transition Focused Abstracts:

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Study on the effect of aqueous phase on CO2 huff-n-puff in tight oil reservoirs and the corresponding stimulation measures.

Authors: Junrong Liu[1]; Hangyu Li[2]; Shuyang Liu[2]; Jianchun Xu[2]; Xiaopu Wang[2]

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CO2 huff-n-puff has been proven to be the most promising enhanced oil recovery method for tight/shale reservoirs. However, the aqueous phase from the connate water and the later-entered hydraulic fracturing has a significant impact on CO2-EOR, and the microscopic mechanism of this effect is still unclear. In this work, an online nuclear magnetic resonance (NMR) instrument was used to monitor the real-time migration of the matrix oil during CO2 huff-n-puff at water invasion conditions. The results show that the intrusive aqueous phase forms a "water bridge"on the fracture surface to prevent CO2 from contacting the crude oil, resulting in poor oil recovery at the first cycle huff-n-puff process. After one cycle huff-n-puff, most of the invasion water in the macro pore will be discharged, and the oil recovery at the second cycle has been greatly improved. However, the water in micropores is still difficult to drive out after multi cycles, which is the main reason why the oil in the micropores is difficult to recover. Increasing the injection pressure can improve the solubility of CO2 in crude oil and increase the elastic energy. Part of the trapped water in the micropore is discharged and the channel is unblocked at the first cycle huff-n-puff, thus improving the oil recovery in subsequent rounds. Similarly, lengthening the soaking period can also significantly enhance oil recovery at the CO2 cyclic huff-n-puff process. The stimulation mechanism is mainly divided into two aspects. One is that invasion water concentrated on the matrix-fracture surface imbibes into the deep part of the matrix during the soaking period, resulting in a decrease in water saturation of the surface, thereby increasing the contact area between CO2 and oil, and finally improving oil recovery. The other is that the invasion water in macropores displaces the oil in micropores under the effect of capillary force, which improves the recovery degree of the micropores.

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Energy Transition Focused Abstracts:

725

Influence of Inertial and Centrifugal Forces on Flow Rate and Patterns of Flow in Natural Fracture Networks

Authors: Stephan Matthai[1]; Heraji Hansika[1]; Cuong Bui[1]; Samintha Perera[1]

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Fluid injection or withdrawal are common in subsurface engineering applications, inducing peak velocities of $\geq$ meters per second in wide-aperture fractures. Although inertia effects are well documented for channel flow, discrete fracture flow models often treat fracture flow as laminar creeping flow or try to account for inertia effects via constitutive relationships. Centrifugal forces acting on the fluid passing through fracture intersections are largely ignored.
This numeric simulation study investigates how flow patterns and spatial variations of flow velocity vary with the total fluid flux through a fracture network. After verification with a fracture intersection model, a Reynolds-averaged Navier Stokes solver is applied to an outcrop-based discrete fracture model, in this sensitivity analysis. Our results show how fluid inertia affects the flow velocity spectra and the partitioning of flow among fractures already at velocities greater than ~1-cm/sec. The significant effects seen, highlight the need for an improved model of fracture flow.

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726

Predicting interfacial tension and adsorption at air-water and NAPL-water interfaces for multicomponent PFAS and hydrocarbon surfactants

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[1] *University of Arizona*

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Per- and polyfluorinated substances (PFAS) are emergent contaminants of which the fate and transport in the environment remain poorly understood. A growing body of site investigations demonstrate that vadose zones serve as significant long-term sources of PFAS to contaminate groundwater. Most PFAS are surfactants and experience strong retention in soils due to adsorption at air–water, NAPL–water, and solid–water interfaces. Notably, a great majority of PFAS-impacted sites comprise mixtures of PFAS as well as hydrocarbon surfactants. The interfacial adsorption of PFAS in

multicomponent systems can complicate the characterization and quantification of retention and mass-transfer processes. Here, we develop a mathematical model to predict air–water and NAPL–water interfacial adsorption for multicomponent PFAS and hydrocarbon-surfactant systems. The model is validated by successful prediction of multiple sets of experimental data covering a wide range of PFAS and hydrocarbon surfactants. The new air–water and NAPL–water interfacial adsorption model can be readily incorporated into transport models to investigate the impact of mixtures of PFAS and hydrocarbon surfactants on PFAS leaching in the vadose zone.

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Energy Transition Focused Abstracts:

MS15 / **727**

Explicit Physics-Informed Neural Networks for Nonlinear Closure: The Case of Transport in Tissues

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[2] *University of Oxford Mathematical Institute*

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In this work, we use a combination of formal upscaling and data-driven machine learning for explicitly closing a nonlinear transport and reaction process in a multiscale tissue. The classical effectiveness factor model is used to formulate the macroscale reaction kinetics. We train a multilayer perceptron network using training data generated by direct numerical simulations over thousands of microscale examples. Once trained, the network is applied in an algorithm for numerically solving the upscaled (coarse-grained) differential equation describing mass transport and reaction in two example tissues. The network is described as being explicit in the sense that the network is trained using macroscale concentrations and gradients of concentration as components of the feature space.

Network training and solutions to the macroscale transport equations were computed for two different tissues. The two tissue types (brain and liver) exhibit markedly different geometry and spatial scale (cell size and sample size). The upscaled solutions for the average concentration are compared with numerical solutions derived from the microscale concentration fields by a posteriori averaging.

There are two outcomes of this work of particular note: 1) we find that that the trained network exhibits good generalizability, and it is able to predict the effectiveness factor with high fidelity for realistically-structured tissues despite the significantly different scale and geometry of the two example tissue types; and 2) the approach results in an upscaled PDE with an effectiveness factor that is predicted (implicitly) via the trained neural network. This latter result emphasizes our purposeful connection between conventional averaging methods with the use of machine learning for

closure; this contrasts with some machine learning methods for upscaling where the exact form of the macroscale equation remains unknown.

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728

Pore network modeling of evaporation in porous media with continuous and discontinuous corner films: corner-network and hybrid pore-network

Author: Ninghua Zhan[None]

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In this paper, corner structure is extracted from real sphere stacking pore structure. Based on the OED-based pore network model proposed in previous study, as shown in the upper left red dashed box in Fig. 1, the corner structure is segmented and the corner network model is constructed, and the corner network and pore network can be coupled. Based on the proposed hybrid network model, the real pore structure was extracted and the evaporation process under isothermal conditions was simulated. The simulation results and experiment results are compared under the overall saturation is 76.6%, 51.6%, 10.1% and 2.9%, respectively. The results show that the distribution trend of local saturation along the thickness direction in the evaporation process is in good agreement. The comparison of liquid configurations on sections with different thicknesses indicates that the position of the residual liquid film in the drying process can be better extracted. Besides, the phenomenon of the edge region evaporating first in the simulation results is inconsistent with the experimental results, which may be due to the lack of considering the physical parameters on the boundary surface.

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Poster / 730

Water transport in n-alkane phases through diffusion and emulsion: insights into oil remobilization from a pore-scale perspective

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Several controlling mechanisms have been proposed to explain oil remobilization due to low-salinity effects. Among them, osmosis and water-in-oil emulsification have been widely reported as two potential mechanisms. However, our knowledge of these processes is limited, and their associated time scales are not well understood. To verify their roles, we have conducted a series of experiments in oil-wet microfluidic devises. The solid surface in the micromodels have been rendered oil-wet via a silanization procedure. Sequential fluid injections with high-salinity water (HSW), pure or surfactant-added synthetic oils, and low-salinity water (LSW) are performed to obtain a fluid distribution where oil is sandwiched between disconnected HSW water and connected LSW. Such fluid distribution is assumed to be prevalent in natural reservoirs. A 2,797 × 2,238 μm2 region is continuously observed for over 70 hours under a high-resolution microscope. We observe that the salinity contrast over oil films can cause water transport through the oil and lead to swelling of the trapped high-salinity water, resulting in the movement of oil phases within the pores. Dodecane displays higher water transport than heptane. We compare salinity contrasts of 1.7-170 g/L and 50-170 g/L. The higher salinity contrast induces higher water transport for both heptane and dodecane. The lower salinity contrast of 50-170 g/L salinity contrast gives less water flux, even reaching zero after a prolonged time. With the addition of a surfactant (SPAN 80) to alkanes, we observe spontaneous emulsification at the LSW-oil interface, while no apparent micro-emulsions were found at the HSW-oil interface. We notice an increase of almost 100 times in water flux for both n-heptane and n-dodecane. This increase is due to the enhanced formation of micro-emulsions of water-in-oil. The emulsification process weakens the influence of salinity on the transport of water molecules in the oil phases. Our experiments provide direct pore-scale observation of dynamic spontaneous emulsification at the LSW-oil interface, whereas we could not detect any micro-emulsions at the HSW-oil interface. Based on our observations, two scenarios for explaining water transport through the oil phase are proposed: water diffusion due to chemical potential gradient and water transport via reverse micelle or micro-emulsions movement. The relative influence of these two transport mechanisms is dependent on the rate of generation of emulsions at the LSW-oil interface, which we observe to be significantly altered by surfactants in the oil phase.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS13 / 731

Confined fluids studied by total neutron scattering

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A lot of processes in applied sciences based on surface chemistry phenomena utilise porous solid materials to increase the accessible surface area. For instance, a mesoporous silica MCM-41 is used as new drug delivery systems for ibuprofen, a more sustainable solution for separation of ethane from natural gas and a heterogeneous catalyst in hydrogenation of benzene. In all of these systems fluid-interface play a key role, however it should be acknowledged that the pores are normally filled up by fluid molecules (i.e. confined fluid).

Nano-confined fluids often have different macroscopic properties than unrestricted bulk corresponding forms. For example, the mobility of molecules is supressed across the whole range of temperatures when liquid benzene is confined in MCM-41.1 Some studies also suggest an interesting phenomena occurring upon confining miscible in bulk mixtures –a microphase separation of e.g. tert-butyl alcohol and toluene.[2] These discrepancies originate at the molecular level, and total neutron scattering is an exceptional experimental technique giving an access to this information.

Wide Q-range total neutron scattering (0.01 to 50 Å−1) accessible at the NIMROD instrument based at ISIS Neutron and Muon Source has been employed to obtain insights into the structural properties of aliphatic and aromatic hydrocarbons such as benzene-d6, cyclohexane-d12, cyclohexene-d10 confined in the pores of MCM-41.[3] Other studies include understanding the structural properties of a range of gases in MCM-41 (oxygen, nitrogen, deuterium, and deuteriated methane),[4] structure of water in MCM-41[5] and arrangement of benzene and cyclohexane molecules during a reaction on Pt-doped MCM-41.[6]

In this study, scattering data were collected for a set of systems: (i) empty MCM-41, and (ii) MCM-41 loaded with a hydrocarbon. To analyse the data, two atomistic models were constructed –first to represent the confining matrix alone, and a subsequent containing also benzene molecules. Through the refining procedure, the molecules within the simulation box were moved towards the new positions allowing for mimicking the collected scattering patterns. The final model of the system is used to calculate structural properties of the confined liquid such as radial and angular distribution functions, spatial density functions, distribution of molecules across a pore.

The results obtained for benzene confined in MCM-41 showed that the some weak interactions that are responsible for 'ordering'of molecules within the bulk liquid benzene seem to be drastically altered by the presence of the constraining interface. The further studies on how the chemical nature of the surface of the confining matrices and their pore size affect the structural properties of confined fluids are ongoing. Understanding the confinement effects on fluids structure is crucial for a conscious tailored design of systems and processes involving them, such as membranes for removal of pollutants from water, systems controlling the fate of drugs within the patients, oil in porous shales, permeable anodes and cathodes in fuel cells and CO2 captured and stored within nano-cages in Metal Organic Frameworks, to name but a few.

Participation:

In-Person

References:

1 Dervin; Queen's University Belfast PhD thesis 2020
[2] Hamid et al.; J. Phys. Chem. C., 2016, 120, 9245
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[6] Hughes et al., Top. in Catal. 2021, 64, 722

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Energy Transition Focused Abstracts:

Poster / 733

Predictions for the porosity dependence of elastic properties and ultrasound wave velocities in isotropic porous media

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Ultrasound wave velocities of porous media are uniquely determined by their elastic properties. In particular, in statistically iosotropic porous media the velocities of the transverse and longitudinal waves can be used to determine the effective elastic moduli and the Possion ratio. On the other hand, many model-based relations have been proposed in the literature to predict the porosity dependence of elastic moduli [1-3], while such relations for predicting the wave velocities themselves are relatively scarce. Especially tricky is the prediction of the longitudinal wave velocity, which is caused by the fact that the porosity dependence of the Poisson ratio is highly non-trivial [4]. In this contribution we present six different model-based predictions for the velocities of transverse waves that can be derived from well-known model predictions for elastic moduli, including the numerical benchmark solutions recently obtained by Pabst and Uhlířová for computer-generated model materials with random microstructure and isometric grains obtained by virtual partial sintering (overlap) of monosized spherical particles [3]. Moreover, we show that a recently introduced velocity ratio function [5] can be used to obtain predictions for the velocity of longitudinal waves as well. It is shown that all these model relations predict a decrease of the wave velocities with increasing porosity, with those based on the Maxwell-Mori-Tanaka model / MMT model being typically highest, followed by those based on the differential, exponential and self-consistent model and those based on the numerical benchmark solution [3] and the Pabst-Gregorová percolation relation [2] being lowest. A comparison with experimental data published in the literature shows that the vast majority of data is between the differential prediction and the aforementioned numerical benchmark solution. Moreover, for all experimental data the correlation between the longitudinal and transverse velocities (both normalized with respect to the transverse velocity of the dense material) is below the MMT prediction and above a straight line with a slope equal to the square root of 7/3.

Acknowledgement: This work is part of the project "Impulse excitation as an unconventional method for monitoring phase changes and microstructural evolution during thermal loading of materials" (GA22-25562S), supported by the Czech Science Foundation (Grantová agentura České republiky).

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS19 / 734

Young's modulus evolution during sintering of ceramics with and without shrinkage

Author: Willi Pabst[1]

Co-authors: Eva Gregorová [1]; Petra Šimonová [2]; Tereza Uhlířová [2]

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Sintering of ceramics consists in the formation of bulk materials from disperse partcicle systems (unconsolidated powder compacts). It always involves strengthening (i.e. due to the formation and growth of sinter necks between the particles or grains) and usually (but not always) also densification (i,e. the reduction of possibly complete elimination of pores) and coarsening (grain growth). During sintering the elastic moduli, e.g. Young's modulus, increase. Using temperature-dependent impulse excitation this has been shown e.g. for alumina ceramics 1, zirconia ceramics [2] and alumina-zirconia composite ceramics [3]. In these cases it is clear that main cause for the increase of Young' s modulus during sintering is the densification which leads to a reduction of porosity and is accompanied by shrinkage. This has been extensively investigated via numerical property calculations on computer-generated model microstructures capturing the essential features of partially sintered ceramics [4-8]. On the other hand, more recently it has been shown that even in cases where sintering occurs without shrinkage, i.e. where the porosity remains unchanged, Young's modulus increases during sintering [9]. The reason for this is the aforementioned formation and growth of sinter necks between the particles or grains, together with changes in the surface curvature of the grains, which may be viewed as a kind of naturally occuring microstructural optimization. This contribution gives an overview on the current understanding of the evolution of Young's modulus during sintering with and without shrinkage. It is shown that apart from porosity, three other Minkowski-functional-based microstructural descriptors can be important in determining Young's modulus, viz.

the surface density, the mean (Germain) curvature integral density and the total (Gauss) curvature integral density. Of these, the surface density seems to be the most influential parameter. Moreover, from the practical point of view, this microstructural descriptor has the advantage that it need not be determined via image analysis but can be determined via gas adsorption measurements.

Acknowledgement: This work is part of the project "Impulse excitation as an unconventional method for monitoring phase changes and microstructural evolution during thermal loading of materials" (GA22-25562S), supported by the Czech Science Foundation (Grantová agentura České republiky).

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 735

A Quick Approach to Model Fault Leakage during CO2 Storage

Authors: Hariharan Ramachandran[1]; Florian Doster[1]; Sebastian Geiger[2]

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Leakage along faults (pre-existing or reactivated) poses a major risk during CO2 storage. Faults and related structures such as micro cracks, joints, fracture networks, deformation bands, fault core etc., can either act as major structural traps or as a connecting pathway to shallow geological layers. Reservoir simulations with an accurate representation of fault-related properties across all scales will help us understand its consequences during CO2 injection and storage. This holds true specifically at an early stage, when the knowledge of storage reservoirs is limited (Availability of high quality well logs, cores and high-resolution seismic are expensive).
This study presents a workflow for ultra-fast screening for fault leakage risk assessment during injection and storage at a concept selection stage. A vertically integrated reservoir model coupled with an upscaled fault leakage function is used for this study. Simulation examples of various injection scenarios in a CO2 storage reservoir with potential for fault leakage are presented in this study. The results show that a good match for CO2 saturation profile is obtained between the fine-scale model and the vertically integrated model at substantially reduced computation time adding confidence for the proposed workflow. Such quick models are extremely helpful in identifying how uncertainties in key fault parameters, reservoir architecture and other constitutive relations affect the storage reservoir behavior and potential fault leakage outcomes for various CO2 injection scenarios.

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Poster / 736

Inertial effects in porous media flow with OpenFOAM

Authors: Damian Śnieżek[1]; Maciej Matyka[2]

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In our poster we will present the complete toolchain for simulating the inertial fluid flow phenomena in pore-scale flows in two and three dimensions based on OpenFOAM (a popular, open–source finite volume code used in computational fluid dynamics).

Our work comprises of specialized python and bash scripts for automating the process of running simulations and post-processing the results. We use the model of high-porosity media that consists of rectangular, random obstacles and examine it in a wide range of Reynolds numbers.

We start by verifying the applicability of the Darcy-Forchheimer laws. Our results confirm applicability of OpenFOAM in simulating high Reynolds flows. Moreover, the energy localization and enhanced channeling effect was also observed. Our study shows that OpenFOAM is a useful tool that allows for relatively easy automation, post-processing, and parallelization of all simulation processes.

Participation:

In-Person

References:

Andrade Jr, J. S., et al. "Inertial effects on fluid flow through disordered porous media." Physical Review Letters 82.26 (1999): 5249.

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Poster / 737

Predicting Representative Elementary Volume by determining the evolution law of the cone of convergence

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To find the effective physical property of a rock, we need to upscale the property from the micro- to the macro-scale. In order to do this process in a correct manner, it is required to find a volume for which the homogenised property does not fluctuate anymore when the size of the sample is increased; the Representative Elementary Volume (REV). Its determination usually comes at the cost of a large number of simulations, since both the value effective property and the size are usually unknown beforehand. On top of that, to resolve with precision the grain in the increasing CT-scan resolutions, the numerical solvers are pushed to the limits, making it overall a computationally expensive process.

Therefore, many scientific studies have been dedicated to optimize the process of finding REV. Using experimental data and numerical methods, the REV has often been related directly to the size of the sample and number of grains within a microstructure, although the REV should depend additionally on the material and physical property of interest. Using statistical numerical methods, research

(Rahman et al, 2020; Mirkhalaf et al, 2016; Kanit et al, 2003) has shown that the fluctuation of the effective property corresponds overall to a cone-like shape convergence.

We suggest determining the generic evolution law of the cone of convergence, which can be used to predict the size of the REV and the effective physical property.

This study is based on simulations of Stokes flow through idealised microstructures (random packing of spheres), unaffected by the natural heterogeneities, from which the permeability is upscaled. By tracing and plotting the convergence of permeability for multiple models, the full cone of convergence appears. This allows us to describe the generic evolution law of the cone of convergence, using a lognormal distribution. The cone shows an exponential growth and decay, converging towards the effective permeability of the sample. It is shown that the rate of convergence depends on the porosity of the sample.

We prove that the determined law of the cone also applies to real microstructures, despite the presence of natural heterogeneities. The importance of this contribution is that we eventually show that it is not necessary to simulate the full sample to find the REV, which is computational expensive, but instead a number of small subsamples is sufficient to predict the size of the REV and the effective property, when the convergence law is known.

Participation:

In-Person

References:

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Unsaturated hydro-mechanical modeling of desiccation cracks in Opalinus Clay

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Co-authors: Gesa Ziefle [1]; Jobst Maßmann [1]; Keita Yoshioka [2]

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At in-situ scale, desiccation cracks might occur in open excavations that remain susceptible to environmental changes such as those related to temperature and relative air humidity variations. Understanding the circumstances under which cracks develop is of great importance in radioactive waste disposal research, since safety aspects related to mechanical integrity and radionuclide transport can be affected by the presence of cracks. In the Mont Terri Rock Laboratory, located in an Opalinus Clay formation in Switzerland, desiccation cracks have been also monitored in the open twin niche of the Cyclic Deformation (CD-A) experiment [Regard et al. 2022]. Within this experiment, several measurements are carried out: water content, suction, crack development, deformation, among others [Ziefle et al. 2021, Ziefle et al. 2022]. The data are combined and/or interpreted with hydro-mechanical numerical models.

We use a hydro-mechanical (HM) model based on a macroscopic poro-mechanical approach that considers partial saturation using the Richards equation [Grunwald et al. 2022, Pitz et al. 2022]. HM coupling is achieved via the effective stress concept, the conservation of fluid mass in a deformable medium and the permeability evolution. We couple the unsaturated HM model with the phase-field approach for brittle fracture to account for shrinkage-induced/desiccation cracking that are strongly influenced by capillary pressure evolution [Cajuhi et al. 2023]. The framework is implemented within the open-source finite element software OpenGeoSys (OGS-6) [Bilke et al. 2022].

In this contribution, we compare the unsaturated HM response of the open twin niche of the CD-A experiment during the winter season, which is a typical desaturation period when the measured relative air humidity inside the excavated niche reduces. We use a set of material parameters obtained from field measurements and literature and compare the model response with the monitored in-situ crack development, for example, air humidity range and capillary pressure under which cracks develop, crack aperture, among others. Furthermore, we evaluate and discuss the influence of an increased permeability on the crack propagation.

Participation:

Online

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Energy Transition Focused Abstracts:

Poster / 740

Montoring the reversible low-to-high-quartz transition and irreversible elastic property changes in sandstone via temperature-dependent impulse excitation

Author: Eva Gregorová[1]

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Temperature-dependent resonant frequency measurements via the impulse excitation technique (IET) can be used to characterize the temperature dependence of elastic properties and to determine the temperature of phase transitions during repeated heating and cooling cycles. In particular, the reversible and hysteresis-free displacive phase transition between the low- and high-temperature subpolymorphs of quartz (low-quartz and high-quartz) involves structural changes that are accompanied not only by changes of density, thermal properties and thermal expansion, but also of elastic properties. On the other hand, polycrystalline quartz-based materials like sandstone (which consists dominantly –but usually not exclusively –of quartz grains), can shift the transition temperature, can introduce a hysteresis of the transition temperature between heating and cooling and can also exhibit irreversible microstructural changes during heating and cooling, which may lead to irreversible changes of elastic properties. In this contribution we present recent results of temperature-dependent impulse excitation measurements obtained for sandstone samples from the Buntsandstein formation at Freudenstadt / Germany (with initial apparent porosities of 12.8 %) from room temperature to 800 ℃ and back (two complete heating-cooling cycles). Using bar-shaped samples it is shown that the low-to-high-quartz transition occurs at around 535 ℃ during heating and at around 560 ℃ during cooling (which is both significantly lower than the single-crystal value of 573 ℃ and clearly indicative of a hysteresis in the transition temperature of quartz in the polycrystalline sample) and that after cooling Young's modulus is significantly lower than before heating, which is a clear indication of damage accumulation (confirmed also by the higher porosity of 14.2 % after cooling). Using disc-shaped samples the temperature dependences of the Poisson ratio and shear modulus are determined in an attempt to answer the intriguing question whether sandstone becomes auxetic in the vicinity the low-to-high-quartz transition, as predicted for single-crystalline quartz 1.

Acknowledgement: This work is part of the project "Impulse excitation as an unconventional method for monitoring phase changes and microstructural evolution during thermal loading of materials" (GA22-25562S), supported by the Czech Science Foundation (Grantová agentura České republiky).

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS20 / 741

A volume-averaged model for acoustic streaming induced by focused ultrasound in soft porous media

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Ultrasound has been found to improve the delivery of therapeutic agents into tumors thereby improving the therapeutic response in cancer treatment 1. Acoustic streaming which is the net movement of fluid generated by propagation of sound waves is one of the many proposed mechanisms for this improvement. However, it would be of great advantage to have an experimentally validated model in order to understand acoustic streaming, and to compare its effect relative to other possible mechanisms for improved delivery.

We have derived equations describing acoustic streaming in soft porous media driven by focused ultrasound. From these equations we created a model that predicts the time-averaged flow on the macroscopic scale as well as the advective transport of the trace components in the fluid. We used this model to perform simulations for different shapes of the focused ultrasound beam. The results from the simulations was also compared to a simplified expression which states that the dimensionless volumetric flux is equal to the dimensionless acoustic radiation force. Finally, we performed a comparison between the model for acoustic streaming to experimental results and we found good agreement, where the predicted volumetric fluxes, averaged over the beam full-width half-maximum, was well within the experimental uncertainties. The hope is that the model can be used to interpret experimental results relevant for enhanced drug delivery in tissue, and to assess the relative importance of acoustic streaming compared with other effects.

Participation:

In-Person

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Energy Transition Focused Abstracts:

743

Remediation of oil drilling cuttings by dielectric barrier discharge plasma

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Co-authors: Stavroula Kavouri [2]; Mary Dourou [2]; Christos Tsakiroglou [1]

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The oil drilling cuttings produced during oil exploration and extraction contain a high percentage of crude oil, ranging from 5 to 20% w/w in dry basis, and must be managed and treated properly before their disposal in environment. Various technologies have been proposed to remediate water and oil-based drilling cuttings such as incineration, thermal desorption, biochemical processes and solidification. Most of these technologies have low efficiency, high-energy requirements and produce secondary pollution. Therefore, it is vital to explore and develop new treatment technologies that would be sustainable, efficient and cost-effective. Non-thermal plasma (NTP) at atmospheric pressure has been successfully applied as an advanced oxidation process for the destruction of organic pollutants present in water and soil 1. During plasma discharges, the collisions between high-energy electrons and cold gas molecules lead to the formation of UV irradiation and highly reactive oxygen and nitrogen species (RONS) able to effectively oxidize and mineralize organic pollutants with low energy requirements [2]. Therefore, NTP is can be regarded as a promising and green remediation technology since no chemical reagents are required. In this study, dielectric barrier discharge (DBD) was investigated as a NTP method for the treatment of oil drilling cuttings. The experiments were performed in a plane-to-grid DBD reactor driven by both sinusoidal and nanosecond pulsed voltage. The performance of DBD technology was determined by measurements of the concentration of the organic pollutants remaining in drilling cuttings after plasma treatment using appropriate chromatographic techniques (GCMS/MS) as well as measurements of the total organic carbon (TOC) which remains in the waste. The effect of DBD operating conditions such as treatment time, applied voltage, energy efficiency, and air flow rate on total organic carbon (TOC) removal in oil drilling cuttings was investigated. The optimum treatment conditions were obtained after repeating the experiments under different values of the operating conditions of the DBD reactor (intensity and waveform of applied voltage, treatment time, gas flow rate, power consumption, etc.) and significant reduction of the TOC (~91%) and total petroleum hydrocarbons-TPH (~99%) was achieved.

Acknowledgements
This research has been co-financed by the European Regional Development Fund of the European

Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH –CREATE –INNOVATE (project code: T1EΔK-02873; project title: "Removal of organic wastes from polluted soils with cold plasma - REMPLASMA").

Participation:

In-Person

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MS19 / 744

Modeling quasi-steady-state phase change transport in polymer electrolyte membrane fuel cells: Effect of surface crack density

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Corresponding Author: pagsalab@ing.uc3m.es

Two-phase transport plays a major role to improve peak power density at low Pt loading in polymer electrolyte membrane fuel cells (PEMFCs). In this regard, optimization of thin porous media of the membrane electrode assembly (MEA) plays an important role to alleviate cathode flooding for enhanced oxygen diffusivity, while maintaining good membrane hydration for high ionic conductivity 1. In this work, the effect of surface crack density of the microporous layer (MPL) on phase change transport is examined by means of a hybrid, multiscale model, which combines continuum and pore network formulations [2-4]. Capillary transport of liquid water driven by phase change is tracked with a discrete invasion-percolation (IP) algorithm, while a standard steady-state continuum solver is used to determine the remaining variables (gas species, dissolved water in the membrane, electronic and ionic potentials, temperature and flow). The coupling of continuum and discrete formulations is accomplished through the incorporation of a control volume (CV) mesh (accounting for heterogeneous effective transport properties) into the continuum-based cell grid. Spatial variations of effective diffusivity, absolute permeability, effective thermal and electrical conductivities and entry capillary pressure are considered. Phase change of water is assumed infinitely fast compared with other transport processes in the MEA (thermodynamic equilibrium), so that condensation/evaporation is governed by the interplay between molecular diffusion of water vapor and IP of liquid water clusters [5]. Therefore, in the quasi-steady-state model, the relative humidity (RH) distribution in the MEA that arises from finite gas diffusion determines the phase change rate of water clusters, which drives the growth/shrinkage of clusters through the path of minimum capillary

resistance. The re-distribution of liquid water during instantaneous IP events in turn modifies the RH distribution. The numerical scheme is stopped when the number of wet CVs does not change anymore because water clusters either reach the channel or approach a nearly zero phase change rate. The interaction between the hierarchical pore structure of the MEA and operating RH and temperature is discussed, with a focus on the effect of MPL crack density.

Participation:

In-Person

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MS20 / 745

Blood-flow simulations in three-dimensional aneurysms using LBM: From risk-assessment to follow-up treatment decisions

Authors: Stephan B. Lunowa[1]; Markus Muhr[1]; Natalia Nebulishvili[1]; Barbara Wohlmuth[1]

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Keywords: Blood-flow simulation, aneurysm, pulsatile flow, porous media, lattice Boltzmann method

Cardiovascular diseases, such as cranial aneurysm or arterial stenosis, rank among the top global causes of death. Therefore, their genesis and treatment are subject of active, interdisciplinary research ranging from medical science via biology, chemistry and physics through to mathematics. Since experimental in-vivo observations are limited and risky for the individual, mathematical modeling and computational analysis facilitate the in-silico assessment of various treatment methods

such as stenting or coiling with patient specific data [3]. For this purpose, we developed a three-dimensional, high-performance computational model for blood-flow simulations through realistic vessel and aneurysm geometries, which are reconstructed from actual MRI-scans. The hemodynamic flow equations include non-Newtonian flow properties for blood characterization and are coupled via the in- and out-flow boundary conditions to a one-dimensional circulatory network simulation 1. We solve the blood-flow model based on the lattice Boltzmann method [2]. Furthermore, we simulate a treatment by coiling using a mechanical wire model to obtain a detailed structural representation. Instead of fully resolving the structure during the flow-simulations, we propose to surrogate it by a porous medium within the aneurysm cavity, so that the interior Darcy-flow is coupled to the vessel's free flow by a generalized Navier-Stokes model. This improves the efficiency of the flow-simulations by allowing for limited resolution. The parameters of the heterogeneous and possibly anisotropic porous medium are found by averaging. We analyzed uncertainties in the parameters and model conditions for relevant quantities of interest. Our numerical results show good agreement between the different approaches. The computational analysis can be directly applied for the risk assessment of aneurysm rupture by evaluation of the resulting wall shear stresses. While the vessel walls are considered to be rigid in previous studies, we aim for a full fluid-structure interaction simulation coupling the blood-flow model to an elastic deformation model of the pulsating vessel wall. Additionally, we envisage the incorporation of a multi-phase thrombosis model on a multi-timescale basis, which could predict the aneurysm occlusion under different treatment regimes.

Funding from DFG, grant numbers WO 671/11-1, WO 671/20-1, gratefully acknowledged.

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Participation:

In-Person

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MS13 / **746**

Dynamics and Phase behaviour of Ionic Liquid Crystal confined in Nanoporous Alumina

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[3] *Hamburg University of Technology and Deutsches Elektronen-Synchrotron DESY*

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Ionic Liquid Crystals (ILCs) are materials that combine the properties of liquid crystals with the ionic conduction similar to ionic liquids. It's known that liquid crystalline mesophases under nanoconfinement exhibit anomalous dynamics and phase behavior. Here, we investigate the dynamics, and phase behavior of a guanidinium based ionic liquid crystal confined in self-ordered nanoporous alumina oxide membrane of pore sizes ranging from 180 nm down to 25 nm using Dielectric Spectroscopy (DS), X-ray scattering and calorimetry. We aim to understand how the pore size and pore surface wettability (hydrophilic or hydrophobic) influence the dynamics, and phase behavior in this system. Our DSC investigations show: (i) the crystalline-liquid crystalline transition decrease with inverse pore diameter and deviates from the Gibbs- Thomson equation. (ii) the liquid crystalline-isotropic transition is completely suppressed for all the confined samples. DS reveals emergence of adsorbed layer process for the ILC confined in native (hydrophilic) pores of 80 and 25 nm, which is absent for the bulk and hydrophobic case, implying the dynamic heterogeneity in the system. We verify the liquid-crystalline –liquid transition using X-ray Scattering and DS. Scattering investigation reveals a change around 130 –140 ℃, where the liquid crystalline order vanishes. Concomitantly, the dielectric relaxation rates exhibit a change around the same temperature limit, implying the liquid crystalline –liquid transition. This liquid crystalline-liquid transition is a Zero-Entropy producing transition, that's unobserved in DSC, and might be unrelated to thermal events. The ionic conduction shows non-monotonic dependence on both the pore size and pore surface chemistry.

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Energy Transition Focused Abstracts:

MS08 / **747**

Surface Induced Anomalous Transport of Nanoparticle in 3D Printed Structurally Heterogeneous Soils: coupling experiments and stochastic models

Author: Filippo Miele[1]

Co-authors: Janis Patino [2]; Veronica Morales [1]

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Fate and transport of colloids and bio colloids in structurally heterogeneous porous media are known to exhibit anomalous behaviours such as non-Gaussian breakthrough curves. Classical approaches, like Colloid Filtration Theory, relies on spatial averaged quantities, neglecting flow topology heterogeneity brought about by both local pore scale surface irregularities and broad pores size distribution: two potential triggers for super diffusive effects and broad trapping time distributions. Recent theoretical work has tried to address these deficiencies by modeling deposition and flow variations as stochastic processes (Miele et al., Phys. Rev. Fluids 2019; Bordoloi et al., Nat. Commun. 2022). However, experimental evidence to demonstrate its validity for 3D geologic structures is still lacking. We thus design a novel experimental set-up to assess colloid fate transport under realistic structural heterogeneity with controlled laboratory conditions. Heterogeneous pore structures are first obtained from X-ray tomography of field samples and are subsequently 3D-printed at high resolution. Column transport experiments with gold (Au) nanoparticles are then conducted at different flow regimes, from which effluent concentration (at the macro scale) and colloid deposition (at the pore scale) are collected. These empirical data are complemented with pore network analysis that parametrizes the co-presence of preferential channels and stagnant cavities and, further, validates the stochastic model of interest. The findings shed light on the main drivers and structural hotspot for colloid filtration in realistic porous media.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 748

Innovating porous materials characterization for hydrogen-storage applications

Author: Mohammad Hossein Khoeini[1]

Co-authors: David Smeulders [2]; Maja Ruecker [2]; Azahara Luna-Triguero [2]

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Multiphase flow and reactive transport in porous media play a key role in various applications needed for establishing hydrogen as an alternative energy carrier. The porous media facilitating the

hydrogen flow in presence of another fluid needs to be optimized in terms of reactivity and transport properties. Two important parameters controlling reactivity and multiphase flow transport in a porous medium are surface area and surface energies in relation to saturation. In this study, inverse gas chromatography is used to correlate surface energy distribution and surface areas at different relative humidity conditions. Due to capillary condensation, the varying humidity conditions reflect a range of saturation. The retention time of probing molecules injected, and the dispersive component of surface energy derived from it, are expected to decrease as humidity increases. The trend for polar/acid-base component of surface energy is not necessarily clear as the interaction of polar probes with water can cause tag-along or displacement effects.

Methodology: Inverse Gas Chromatography
Inverse gas chromatography (iGC) has been reported as a powerful, sensitive, and relatively fast technique for characterizing the physicochemical properties of porous media such as BET surface area and energy distribution of the surface 1. In this technique, a single gas, known as probe molecule, is injected into a column packed with the porous sample under investigation. The probe molecules pass through the column, interact with the porous material, and the retention time of the probe molecules is measured at the end of the column. Measuring the retention time for different probes, e.g. polar and non-polar, enables us to determine a wide range of physicochemical properties of the porous material.

Discussion: Measurement in humid conditions
Recent advances in commercial IGC enable users to perform accurate experiments at different humidity. The water molecules' presence in the system initially adsorb on high-energy sites of the surface and gradually change the surface area of porous material exposed to other components in the system [2]. By measuring surface energy at different relative humidity, one can correlate the surface area to surface energy. In practice, the presence of water in the system would hinder the adsorption of probe molecules, depending on intermolecular forces between them, known as a tag-along effect [3], and/or competition in adsorption. In the case of using non-polar probes, e.g. n-alkanes, it is expected to see a decline in retention time, surface area, and the dispersive component of surface energy as humidity increases. This is due to the fact that water molecules will interact with high-energy sites on the surface, covering part of it (figure 1). In the case of polar probes, used for the determination of polar or acid/base components of surface energy, the trend is not clear. Interaction between water and polar probes is stronger than with non-polar and may cause the formation of a cluster or concentration-dependent displacement effects. In this study, we assess the effect of water in the determination of surface area and surface energy by IGC, parameters which control multiphase flow and reactive transport in porous media.

Participation:

In-Person

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Poster / 750

Structural controls on the development of karst environments: A multi-scale experimental investigation

Author: Théo BRIOLET[1]

Co-authors: Elisabeth BEMER [2]; Olivier SISSMANN [2]; Jérôme FORTIN [3]

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About 25% of the global population depends on karst groundwater. It is therefore essential to better understand the genesis and development of karst environments. Karst landscapes are shaped by multiple physical and chemical processes that occur over thousands to millions of years, the dominant one being the dissolution of soluble rocks like limestone or dolomite. This process strongly depends on the partial pressure of acidifying gases like CO2 in the atmosphere, the soil type, and the presence of faults in geological formations. Although karstification and rock dissolution are natural processes, they are strongly influenced by anthropic activities, especially air and water pollution, as well as land use.

The aim of this study is to better understand the dissolution kinetics and especially its control on dissolution patterns determination. To do so we developed a multi-scale experimental protocol based on dynamic alteration of rock samples. Coreflood experiments were performed on 80 - 100 mm long core plugs (core plug scale - cm) and micro-coreflood experiments were performed on grounded samples (rock powder scale - µm). In the coreflood experiments, CO2-saturated water was injected at a flowrate of 140 cm3/h for 5 days, under 30 bar confining pressure and at room temperature. The petrophysical properties of samples were measured, and CT scanner imaging, SEM observation and BET analysis were performed before and after the coreflood experiments. Micro-coreflood experiments were performed on different grain size powders using chromatography columns. These experiments were designed to study dissolution kinetics for multiple grain sizes and thus deconvolute the structural and chemical impacts. For both coreflood and micro-coreflood experiments, chemical concentrations of dissolved species were determined using ICP-AES.

Two carbonate rocks are considered: Euville crinoidal limestone (Phi=12-18%, k=10-150 mD) and Lavoux oolitic limestone (Phi=20-30%, k=100-300 mD). Both limestones have similar mineralogy (99% calcite) and a bimodal porosity distribution, but their microstructure is significantly different. Despite their higher porosity and permeability, Lavoux samples show a larger fraction of micropores. Choosing these samples allow to investigate microstructural effects on dissolution processes regardless of major chemical compositions variations.

For coreflood experiments, CT Scanner imaging shows that dissolution patterns in Lavoux limestone are dominated by the development of localized dissolution channels (”wormholes”); whereas dissolution in Euville limestone appears more diffuse. Mean porosity increased by around 4% for Lavoux samples and 2-3% for Euville samples, while permeability increased by at least 10 and 35 times respectively. Core plug-scale results show that higher mean dissolution rates for Lavoux samples.

BET analysis and SEM observations show that the higher dissolution kinetics of Lavoux limestone is mainly related to a larger specific surface area leading to a higher reactivity. The difference in dissolution kinetics between Lavoux and Euville limestones is still present in the micro-coreflood experiments, but it decreases with grain size, revealing a specific structure for each limestone even at the powder scale. These results suggest that the specific surface area of the microporous grains is a key control parameter for larger scale dissolution .

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS01 / **751**

Microfluidic hydrogen storage capacity and residual trapping during cyclic injections

Author: Maksim Lysyy[1]

Co-authors: Na Liu [2]; Celine M. Solstad [1]; Martin Ferno [1]; Geir Ersland [3]

[1] *University of Bergen*

[2] *University of bergen*

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Underground hydrogen storage (UHS) in porous media offers a long-term and large-scale storage solution which is vital for a sustainable H2 economy. Despite growing interest in the topic, the understanding of the physical processes during cyclic H2 flow is not yet adequate. Here we use microfluidics to experimentally investigate multiple cycles of H2 injection and withdrawal under a range of injection rates at shallow reservoir storage conditions. Our analysis is aimed at qualitative and quantitative description of H2 reconnection mechanisms and hysteresis. We find that H2 storage capacities increase with increasing injection rate. The residual H2 saturation is reproducible between cycles, but its distribution in the pore space visually appears to be hysteretic. In most cases, the residually trapped H2 reconnects in the subsequent injection cycle, predominantly in proximity to the large pore clusters. Our results provide valuable experimental data to advance the understanding of multiple H2 injection cycles in UHS schemes.

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In-Person

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MS18 / **752**

On clean-up of iodinated X-ray contrast media agents from surface waters

Authors: Stefano Seccia[1]; Mohaddeseh Mousavi Nezhad[2]

Co-author: Gustave Denis [1]

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Iodinated X-ray contrast media (ICM) agents are a class of pharmaceuticals and personal care products (PPCPs) of growing concern in environmental science as emerging contaminants [1, 2]. ICMs are the primary source of adsorbable organic iodine responsible for the formation of iodinated disinfection byproducts (I-DBPs), highly toxic compounds commonly found in surface waters [3]; as such, prevention and remediation strategies are necessary for the removal of these contaminants from natural waters [4, 5]. Nonetheless, there currently does not exist a scalable, environmentally safe, and efficient strategy for their removal from natural waters. Adsorption systems are routinely used in water treatment and purification from contaminants, and have the major advantage of preventing the formation and release of toxic byproducts [6]. In addition, adsorption of ICM agents to potential absorbents is an approach for purification of water resources from this emerging contaminant. To this end, studies investigating the sorption dynamics of these compounds to candidate sorbent materials, in different experimental conditions, are needed.

In the present study, the adsorption capacity of the non-ionic ICM iopamidol and the ionic ICM diatrizoate onto candidate sorbent materials has been investigated by means of single sorption batch tests, under both equilibrium and kinetic conditions. Column tests have also been performed to highlight the influence of contact time and dynamic flow conditions on the sorption process, with experimental conditions selected based on their relevance for field applications.

In batch equilibrium tests, neither ICM agents showed sorption to soils, thus highlighting their peculiar nature as non-lipophilic contaminants remaining in the water phase [7]. A novel iron oxide-based colloidal suspension was also incapable of removing the target compounds, thus highlighting the need for sorbent materials with specific characteristics. A pelletized activated carbon sorbent material was successful in removing the target ICM agents in different experimental conditions. Effect of a variety of influencing factors such as amount of sorbent and sorbates, contact time, and hydrodynamic condition on the removal rate of the ICM agents were analysed. The results, gathered with the aim of understanding the key principles and dynamics behind ICM agents adsorption, offer a new set of data that inform one how to design tailored removal strategies and industrial treatment processes.

Participation:

In-Person

References:

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MS01 / **753**

Underground hydrogen storage and in-situ gas conversion: macroscopic investigation on reactive transport mechanisms

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[1] *Montanuniversität Leoben*

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The bulk of renewable energy production varies in a way that typically does not align with time-dependent energy consumption. This can lead to an energy surplus or a shortage of the energy supply causing a challenge in supporting the baseload requirements. Enormous storage capacity is required to accommodate these fluctuations in supply and enable large-scale storage of excess renewable energy. Gas as chemical energy carrier, and hence energy, can be stored in such large amounts in subsurface structures of depleted reservoirs. Especially hydrogen gas is an excellent energy carrier and can be produced via electrolysis from the surplus of renewable energy.

First pilot tests in the field were carried out to estimate the risks of hydrogen loss and a reduction of the stored energy due to physical, chemical or biological processes. It turned out that most notably microbial processes lead to a decline of hydrogen and hence to loss of energy. In these processes, microorganisms convert hydrogen and carbon dioxide into methane. This observation, which is detrimental in terms of hydrogen storage security, yield to a new approach to efficiently store excess renewable energy in the form of "renewable"methane. Such operations include a (possibly cyclical) usage of CO2 and can therefore be treated as CCU projects (Carbon Capture and Utilization). The possibility of using these processes as in-situ bioreactor to generate and store "renewable"methane is investigated. The biochemical reactions which convert the gases also lead to a growth of biomass in the pore space. The expansion of biomass will reduce the available pore space for gas storage and likely the permeability of the reservoir rock as well. Consequently, biomass may compromise storage capacity and injectivity substantially.

This work aims to investigate crutial processes of the in-situ methanation on different time and length scales containing numerical simulations and laboratory experiments. With core flooding experiments on the meter scale, we want to get a macroscopic insight into the reactive transport mechanisms which are governing (a) the hydraulic properties, and (b) the gas conversion rate and hence the overall performance of the subsurface reactor. Numerical field scale simulations are used to study the dynamics of the macroscopic conversion process under assumptions concerning conversion rates and field geometries. By using simplified models, mechanisms are identified and their performance is investigated by sensitivity analysis. The approach is to perform generic field scale simulations in order to understand the flow and reaction kinetics and their coupling.

The aim of the presented study is to develop a workflow that contains both, numerical and experimental components to gain a holistic understanding of the physical and biochemical mechanisms of the in-situ methanation. With the resulting comprehensive datasets, we expect deep insights into bio-reactive hydrogen transport and the controlling parameters to be applied to future field cases.

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Poster / 754

Experimental study of microbial effects on anhydrite and cement during hydrogen storage in salt caverns.

Authors: Joyce Schmatz[1]; Garri Gaus[2]; Fabien Georget[3]; Jop Klaver[4]; Saeed Khajooie[2]; Hendrik Ballerstedt[5]

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[3] *Institute of Building Materials Research, RWTH Aachen University*

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Although a number of studies have been carried out, especially in recent years (e.g., Hemme and van Berk, 2018), to evaluate the chemical-physical influences of hydrogen storage in underground salt caverns, many questions still need to be answered. Because of the lack of reliable data on the effect of hydrogen on permeability and mechanical integrity in the critical lithologies, such as anhydrites, sump sediments, or the casing cements, as well as information on the kinetics of abiotic geochemical and microbial reactions in the corresponding pore fluids, predictions on the long-term behaviour of geological hydrogen storage are only possible to a limited extent. For this, knowledge about the volumetric extent and kinetics of the reactions is essential. Experimental work and microstructural analyses is required to determine the input parameters for the geochemical models on the different reaction kinetics.

We will present the first results of an experimental study demonstrating kinetics of biotic and abiotic reactions of H2 and H2S with anhydrite and casing cement, taking into account for instance the bacterial growth and reduction rate, the brine volume and sulfate concentration, pressure and temperature. Our objective is to visualize the known but also the unknown processes occurring, which may affect the mechanical integrity of salt cavern during hydrogen storage at various scales, by microstructural analyses. It can be assumed, that the reactions are challenging to constrain in a laboratory experiment due to slow rates, however, microstructural investigations allow the determination of the onset and development of the chemical alteration of the materials already at a relatively early stage down to the submicron pore scale.

In the first step, the sample material (anhydrite and cement) was investigated using a range of established microanalytical techniques and methods to assess the microstructure, pore space and mineralogy at high resolution and accuracy (e.g., Klaver et al., 2015, Jiang et al., 2021). Considering the low permeability, of anhydrite/polyhalite, these samples were artificially fractured before assembly

in the flow cell to enlarge the surface area. The experiments are designed in a way, that they allow assessing the effect of biomass accumulation on hydraulic conductivity, as well as the bacterial sulfate reduction. After completing the investigation, microbial activity, changes in pore space due to biofilm formation, and the mineralogical changes in the solid phases were studied ex-situ using scanning electron microscopy on the sample surfaces polished with a broad ion beam under cryogenic condition (Schmatz et al., 2015, Pötschke et al., 2022). The method enables the visualization (of the onset) of the biological, chemical and structural changes in the sample material and opens up the possibility for upscaling the processes.

Participation:

In-Person

References:

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The KEM program of the Dutch Ministry of Economic Affairs and Climate is kindly supporting part of this research.

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MS16 / 755

Towards the Print Excellency via Ink –Media Interactions Ideation

Author: Nicolae Tomozeiu[1]

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Corresponding Author: nicolae.tomozeiu@cpp.canon

The inkjet technology fuels the rapidly evolving world of printing. This printing technology delivers good print quality using the flexibility of digital printing at a breakthrough cost price. The R&D

department of Canon Production Printing company, is a major player in the development of inkjet technologies for many different applications.

The physical processes which regulate the interactions between a sessile droplet and a thin porous paper have been the subject of many studies in the last decades. Both theoretical understanding and sustainable industrial applications are the driving forces for these studies.

Liquid spreading, evaporation and imbibition into porous material are physical processes that describe the interactions of aqueous ink with paper. Understanding them is vital for having prints of high quality; and this is the aim of this work. The influence of the liquid ink physical properties as well as of the paper characteristics are considered. Experimental studies based on Optical Spectroscopy & Microscopy, Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance (NMR), Electrical Impedance Spectroscopy (EIS), High Speed Camera Recordings (HSCR) and Automatic Scanning Absorptometer (ASA), are presented revealing the three main physical phenomena that dictates droplet dynamics: spreading, evaporation and absorption. Theoretical models and results of computational simulations are strengthening the analysis of the experimental results.
Besides the liquid part, the investigated complex fluids contain particles (pigment and colloidal polymeric latex). The result of drying process is an ink solid thin film formed onto porous paper with optical and mechanical properties. Targeting the print excellency, this work provides an extensive overview of the methods to investigating the interaction between ink and paper, highlighting their strengths and limitations.

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In-Person

References:

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Energy Transition Focused Abstracts:

MS09 / 756

Analysis of CO2 trapping potential by combining morphology-based digital rock simulations and pore-scale flooding experiments

Authors: Bianca Brandstätter[None]; Pit Arnold[1]; Holger Ott[2]; Rene Ritter[None]; Lobel Danicic[None]

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In the eye of climate change, Carbon Capture and Storage (CCS) gained importance as a large-scale option to permanently sequester CO2. To ensure storage safety, it is crucial to understand trapping mechanisms and the trapping potential. To do so in a time-efficient way, the application of Digital Rock Physics Simulation has become a major tool. The presentation will focus on capillary trapping by re-imbibition simulated by means of the morphological approach and benchmarked by pore-scale flooding experiments.

Using the data of flooding experiments with in-situ pore scale imaging, fluid configurations in digital twins of various sandstone samples were simulated and compared to experimental results. To compute the trapping potentials of those rocks, simulations of primary drainage and subsequent imbibition processes were performed based on the morphological method. From the results, land trapping model constants were calculated depending on the initial and residual CO2 saturations of the imbibition processes. For obtaining realistic results, we make use of recent developments in the frame of the morphological approach in digital rock physics by Arnold et al. Prior to that, only spontaneous imbibition processes could be simulated, now extended to the whole imbibition branch including forced imbibition. Also, the effect of wettability and contact angle variation is considered in a stochastic and deterministic way. Simulations of multiple scenarios with varying input parameters were performed to benchmark against experimental results and as first step towards stochastic input for reservoir modeling.

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In-Person

References:

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MS05 / **757**

Biofilm growth in heterogeneous porous media: pore-scale modeling and anomalous transport analysis

Author: Xueying Li[None]

Co-authors: Xiaofan Yang [1]; yurong yang

[1] *Faculty of Geographical Science, Beijing Normal University*

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Biofilms are complex microbiome in extracellular polymeric substances that regulates the biological environments in porous media. The phenomenon of solute anomalous transport can be induced from the evolution of biofilm which dynamically alters the pore structure, the hydrophobicity, and the hydrological-biogeochemical processes in the pore space. So far, few study has pay attention to scaling the regime of biofilm-induced anomalous transport through numerical modeling and simulation. In this study, an in-house developed solver BioFOAM, based on the micro-continuum theory and the Darcy-Brinkman-Stokes equation, was developed to simulate pore-scale solute transport of fluid flow and biofilm growth. Parameter sensitivity analysis were then conducted to investigate the effects of the substrate concentration (c), the Monod kinematic parameter (ks), and the growth rate (μ) on transport properties. Finally, anomalous transport regimes were quantified via breakthrough curves under different Reynolds (Re), Peclet (Pe) and Damköhler (Da) numbers. Results revealed that (1) the biofilm growth process significantly altered the flow velocity field by reshaping the pore structure and forming recirculation zones. These behaviors resulted in the evolution of solute transport pathways in heterogenous porous media. (2) The parameter c, ks, and μ demonstrate different

sensitivities towards biofilm growth processes. The growth rate was the most sensible parameter. The biomass density, the averaged porosity and permeability varied significantly even at the value of 10^{-6}. The Monod kinematic parameter showed a clear dividing region from 10^{-3} to 10^{-4}. When *ks* was below 10^{-4}, the biomass density accumulated while the porosity and permeability decreased. When *ks* was larger than 10^{-3}, the biofilm growth was invalid. The substrate concentration was not sensitive for biofilm accumulation. (3) The nondimensional number Da was useful in analyzing anomalous transport regimes, while the variation of Re and Pe did not bring much difference to the breakthrough curves. For the case of biofilm growth on a single grain, the valid anomalous breakthrough regime was within the Da from 0.018 to 0.054. When Da was below 10^{-3} or above 10^{-1}, the anomalous breakthrough phenomenon disappears. For the case of biofilm growth in heterogenous porous media, the valid anomalous breakthrough regime was within the Da from 2.5×10^{-4} to 3×10^{-3}. When Da was as small as 1.5×10^{-4}, the anomalous breakthrough phenomenon disappears. When Da was as large as 6×10^{-3}, the numerical experiment received numerical error. In general, when the Da number was within the anomalous transport regime, the characteristic time decreased and the tails stretched longer as the increase of the Da number. This study provides a specific modeling case to analyze the biofilm-induced anomalous transport regimes, which can be regarded as a comparative effort to theoretical studies on the scaling of anomalous transport regimes.

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Energy Transition Focused Abstracts:

MS08 / **758**

Effect of radial advection on chemical fronts

Authors: Anne De Wit[1]; Alessandro Comolli[2]; Luka Negrojevic[3]; Fabian Brau[4]

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The reaction-diffusion-advection properties of chemical fronts are studied both theoretically and experimentally in the case where one reactant is injected radially into the other reactant at a constant flow rate. At long times or equivalently large radius from the injection point, the properties of one-dimensional reaction-diffusion fronts are recovered as the influence of the advection field decreases radially. However, at early times i.e. for a smaller radius, advection plays a crucial role. We characterize the influence in this transient regime of the injection flow rate and of the ratio of initial concentration of both reactants on the position of the front, the reaction rate and the amount of product generated. We discuss the role of the kinetics of the reaction on the possible accessible regimes. We confirm experimentally the theoretical predictions in polar geometries using either simple A+B->C reactions or the autocatalytic chlorite-tetrathionate reaction.

Participation:

In-Person

References:

A. Comolli, A. De Wit, F. Brau, "Dynamics of A + B ⟶ C reaction fronts under radial advection in a Poiseuille flow", Phys. Rev. E 104, 044206 (2021).
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Energy Transition Focused Abstracts:

MS09 / **759**

Meshless Lattice Boltzmann Method for pore-scale porous media flow and parameters calculation

Authors: Dawid Strzelczyk[1]; Miha Rot[2]

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Lattice Boltzmann Method (LBM) has for long now been successfully used
as a numerical tool for modeling fluid flow 1. This is due to the local treatment of nonlinear parts of the algorithm, the ability to model non-trivial particle interactions in a bottom-up manner, the potential for parallelization, and the ease of implementation. However, applied to complex geometries often encountered in pore-scale porous media research, the inherent feature of LBM - the necessity to operate on square grids - makes the appropriate boundaries discretization and local grid refinement a difficult task. Supplementing the standard, lattice approach with meshless interpolation can bring several advantages, including the ability to operate on discretizations consisting of non-connected nodes with non-uniform spatial density, more accurate boundaries representation, and decoupling of velocity and space discretization. In consequence, combining LBM and meshless interpolation has a perspective to result in an efficient, robust, and flexible numerical method for modeling flow in complex geometries.

In the talk, an application of meshless LBM for the calculation of permeability and drag coefficient will be presented along with a comparison with standard LBM and meshless Navier-Stokes solver results. Special attention will be given to the impact of boundary conditions implementation and hydrodynamic force calculation method on the accuracy of the results. Idealized and real porous samples will be considered.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 760

Numerical investigation of chaotic advection in porous media at the Pore and Darcy scales

Author: Stefano Ascione[None]

Co-authors: Tanguy Le Borgne [1]; Daniel Lester ; Guillem Sole Mari [2]; Joris Heyman [3]

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[2] *University of Rennes, University of Notre Dame*

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Solute transport in porous media plays a significant role in industrial and natural processes, since porous materials are ubiquitous on Earth. Modelling transport is important for various applications, including soil moisture dynamics, groundwater pollution, and oil recovery. Previous research suggested that chaotic mixing 1, e.g. the exponential elongation of fluid elements by advection, strongly depends on lattice geometries, flow direction [2] and packing density [3]. However, a universal understanding of chaotic advection at Pore and Darcy scales is still missing. Here, we present a numerical study of 3D Pore and Darcy scale flows through various representative elementary volumes. In this instance, we consider the impact of impermeable inclusions on the mixing dynamics of homogeneous Darcy flow. We computed Stokes and Darcy velocities for constant pressure gradient in mono-dispersed bead packs with body-centered cubic (BCC), face-centered cubic (FCC), and random lattices. By computing periodic trajectories, we then estimate the magnitude of the largest Lyapunov exponent in all these flows fields, and compare them with a new predictive model. Our results provide original perspectives on the control of chaotic mixing by the porous structure.

Participation:

In-Person

References:

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Micro-Scale Characterization of Nanoparticles Adsorption onto Oil-Water Interface and Stripping Capacity of Oil Film: Effect of ”Ship Anchor ”

Author: Mingliang Han[1]

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Nanofluids have been widely employed to enhance oil recovery in low permeability reservoirs due to their excellent interface regulation performance. It is of great value to characterize micro-scale behaviors of nanoparticles adsorption and their stripping capacity of oil film, that is the theoretical basis for defining the principle of nanofluids enhancing oil recovery and guiding the synthesis of nanoparticles.

For this pupose, molecular dynamics simulations were employed to investigate the adsorption behavior of SiO2 nanoparticles with different modifications of surface design and the ability of them to reduce the interfacial tension. The results show that the types of modified groups, the density of modified groups, and the length of alkane molecular modified on the nanoparticles affect the wetting state of nanoparticles at the oil-water interface. As the alkane molecules onto nanoparticle surfaces become longer and denser, the Van der Waals between the nanoparticles and the oil film is stronger. Unsaturated oxygen on SiO2 nanoparticles surface and the modified hydrophilic groups (such as carboxyl group, amino group, etc.) cause strong Van der Waals interaction and hydrogen bond between nanoparticles and water molecules. The ionization of modified groups generates electrostatic interaction with ions in the water phase. Therefore, the integrated interaction among water/nanoparticles/oil determines the contact angle of nanoparticles onto the oil-water interface. In addition, the factors mentioned above also generates different capabilities to reduce interfacial tension, which is most sensitive to the length of the modified alkane molecule.

In addition, the micro-mechanical behavior analysis among oil, water and nanoparticles during nanofluid flooding is quantitatively characterized. Without nanoparticles, the water cannot drive oil film when flowing on its surface due to the weak force between oil and water molecules. The adsorption of nanoparticles onto the interface could help the water drive the oil film and then peel off the oil film from the pore surface due to the strong attraction between the water and hydrophilic part of nanoparticles, and the oil and hydrophobic part of nanoparticles. As a result, nanoparticles play the role of “ship anchor” to strip oil film. Significantly, the short range of intermolecular forces leads to the limited mechanical action thickness of nanoparticles. The factors affect the action thickness of nanoparticles were investigated. The optimal contact angle and nanoparticle size with the best flooding effect for oil film with different thickness and composition were achieved. The work provides theoretical guidance for the synthesis of nanoparticles.

Participation:

Online

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Energy Transition Focused Abstracts:

MS08 / **762**

Effect of evaporating surface to volume ratio on crystallization dynamics and damage caused by NaCl crystallization in porous media

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Understanding the dynamics of salt crystallization in composite materials where an interface between two porous media with different material properties is present, is of paramount importance to understand the decay mechanisms involving such crystallization. Often the crystallization will cause cracks in the material that can act as an additional evaporating surface. As a result the surface to volume ratio of the material changes, which can create a different type of crystallization, resulting in a different damage mechanism. This problem is relevant to the practice of art conservation and for many salt crystallization problems in civil engineering.
Over the past decades, much has been learned about the effects of salt crystallization within a single type of homogeneous porous material. In order to investigate the more complex situation of layered porous materials, the European JPI-CRYSTINART project was initiated in 2020. Our investigations within this project focus on the influence of surface to volume ratio on the evaporation of NaCl solutions in cone-shaped sandstone samples and the resulting efflorescence and damage caused by salt crystallization. For this purpose, we designed truncated cone-shaped materials saturated with aqueous 10wt% NaCl solutions. The cones only dry from the top surface (the sides and bottom surface were sealed off), and drying experiments were performed with the small or the large cone surface facing upwards.
In the experiments, the drying kinetics and dynamics of salt precipitation (NaCl) are investigated

in real-time by simultaneously using optical microscopy with automated image analysis and mass change registration during the evaporation. Additionally, we performed combined H and Na profile NMR experiments to measure the advection and diffusion of the salt ions within the cone shaped samples during drying. Laser profilometry has been also used to get information on the salt crust at the top surface. Our results reveal that the surface to volume ratio has a large influence on the drying dynamics but also on the way the salt crystallizes. The small surface to volume ratio shows an exponential drying regime and exhibits a large amount of efflorescence (salt crystallization on the surface) with a fractal appearance. The fractal salt deposit lifts itself up away from the sample surface due to the formation of tiny salt pillars at the end of the drying; consequently, the salt crust can easily be removed from the sample surface or even falls of by itself. To the contrary, the high surface to volume ratio exhibits a linear drying regime and causes a different type of efflorescence which adheres strongly to the surface of the porous stone without a self-lifting behaviour
The surface to volume ratio therefore plays a major role in both the drying and crystallization dynamics of a salt solution in a porous medium. Understanding these principles could help to elucidate the mechanisms of different types of efflorescence in relation to the evaporation speed and resulting ion transport in the porous medium, in order to propose solutions to prevent salt damage or to come to better conservation strategies.

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Energy Transition Focused Abstracts:

Poster / 764

Gas trapping mechanism and the potential impact on productivity of geothermal reservoirs

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Entrapment of the non-wetting phase in porous media has been observed in a variety of fields such as petroleum engineering or geological storage of carbon dioxide. Our study aims to monitor gas trapping under in-situ conditions using X-ray computed micro-tomography to evaluate gas trapping as a possible mechanism for a decreasing productivity index of geothermal reservoirs. The transient behavior of the productivity index in the test site of Groß Schönebeck (north of Berlin, Germany) indicates irreversible changes of the reservoir characteristics caused e.g. by scaling's or the accumulation of free gas and/or fines due to changing mechanical loads i.e. changes of pressure and temperature (Blöcher et al. 2016). Typically, these gas bubbles can migrate upward due to buoyancy, but while they grow in size they may get trapped in the pores (Mahabadi et al. 2018). Consecutive X-ray computed tomography (CT) scans of a typical siliciclastic rock were generated while the pressure was decreased stepwise to mimic gas bubble generation. The cylindrical sandstone core

with a diameter of 5 mm was coated with a viton-sleeve and positioned inside a self-manufactured core-holder design made from aluminum and resin using stereolithography 3-D printing (SLA) for prototype production. The cell is placed inside a μCT scanner with a 225 kV multifocal X-ray tube for high resolution X-ray tomography resulting in a resolution of about 6 μm. A scan of the sandstone with a porosity of about 10 % was gathered after nitrogen was injected to the core. Further images were obtained after water injection at pressures up to 4 MPa. The scanning procedure was repeated after flow through experiments with flow-rates of 2 ml/min were carried out for an hour each. Images were analyzed using the software Avizo Fire, Version 9.0.1©. The images were filtered in 3D with an edge preserving non-local means filter and binarized using a modified Otsu thresholding procedure (Otsu 1979). Further quantification algorithms were implemented in Phyton. A pore-network model was extracted from the three-dimensional data and will be used to evaluate the changes in hydraulic conductivity at each timestep. The distributions of the volume of trapped gas bubbles is estimated from the scanned images by subtracting the timesteps from the fully water saturated sample to highlight changes in density. The trapped gas fluctuates and generally higher trapped gas saturation is observed in larger pores and the more porous layers. This results in a clear reduction of permeability that could potentially explain the decreasing productivity index observed in several geothermal sites.

Participation:

In-Person

References:

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Poster / 765

Pore-scale imaging and analysis of surfactant flooding

Author: Hussain Alzahrani[1]

Co-authors: Branko Bijeljic [2]; Martin Blunt [3]

[1] *Hussain*

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Carbonate reservoirs account for most of the global daily oil production and hold more than half of the world's total proven conventional oil reserves. Surfactant flooding is one promising improved oil recovery technique to maintain production from mature carbonate reservoirs.

We apply three-dimensional pore-scale imaging and analysis at representative reservoir conditions to observe and interpret the mechanisms of improved recovery during surfactant flooding. The work can be used to improve the assessment and design of improved oil recovery in carbonate formations. We focus on low-concentration surfactant injection where the likely mechanism for improved recovery is a wettability transition towards more water-wet conditions. We study recovery using cationic surfactants. They have positive charges on their heads and are considered the best candidate for carbonate rock wettability alteration.

We investigate fluid displacement, oil recovery, and quantify in situ changes in wettability when a cationic surfactant, DTAB, is injected into a cm-scale carbonate rock sample. X-ray microtomography along with sophisticated image processing software is used to acquire, process, and analyse the images. The interfacial tension between brine and oil, and between the surfactant-laden aqueous phase and oil is measured to determine the impact of interfacial tension on wettability alteration and recovery. The phase behaviour and nature of any emulsion formed is also quantified.

The rock sample is a Estaillades limestone core which undergoes crude oil injection for three weeks at a high temperature to reach a representative reservoir wettability state. Then, the brine is injected to represent secondary waterflooding. Finally, the surfactant is injected as a tertiary recovery method. High-resolution images were used to quantify the fluid configuration in the pore space. Wettability is quantified and characterized by measurements of in situ contact angles and curvatures.

The outcome of this work is to establish a methodology in which high-resolution 3D imaging using X ray micro tomography can be combined with surfactant flooding in secondary or tertiary mode to quantify in situ changes in wettability and to elucidate micro-scale fluid displacement processes. This work furthers our understanding of oil recovery mechanisms when a cationic surfactant is used as a secondary or tertiary enhanced oil recovery process.

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In-Person

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Poster / 767

Soil texture linking saltwater intrusion in coastal regions to surface soil salinity

Authors: Vahid Sobhi Gollo [1]; Eva González [2]; Jörg Elbracht [2]; Peter Fröhle[3]; Nima Shokri[1]

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The sea level has risen notably in recent decades compared to the most recent millennia. This exposes coastal areas to hazards ranging from enhanced flooding and erosion to groundwater contamination and soil salinization referring to excess salt accumulation to a degree that adversely influences soil and environmental health (Hassani et al., 2020, 2021). This study focuses on how soil properties modify the near surface salt accumulation as a result of saltwater intrusion in coastal regions. To do so, we developed a predictive model, using software package FEFLOW, capable of describing the effects of soil texture and heterogeneity on the surface soil salinity as a result of saltwater intrusion through the unsaturated zone. For model validation, we used the field-scale data measured in "Alte Land"located in north Germany - an agriculturally significant area threatened by the increasing soil salinity. After the model verification, we conducted hypothetical numerical experiments to identify how soil texture, linking saltwater intrusion through unsaturated zone to the surface, influences surface soil salinity under different boundary conditions. Our results show how significant could be the changes in surface soil salinity as a result of minor changes in soil texture and heterogeneity. This highlights the importance of soil characteristics on surface soil salinity driven by the saltwater intrusion in coastal regions with the results relevant to soil health and land management in coastal regions.

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References:

Hassani, A., Azapagic, A., Shokri, N. (2020). Predicting Long-term Dynamics of Soil Salinity and Sodicity on a Global Scale, Proc. Nat. Acad. Sci., 117 (52), 33017-33027.

Hassani, A., Azapagic, A., Shokri, N. (2021). Global Predictions of Primary Soil Salinization Under Changing Climate in the 21st Century, Nat. Commun., 12, 6663.

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MS14 / 768

Techniques for the estimation of hydrogeological parameters in a cluster of infiltration ponds

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Identifying the final fate of treated wastewater is sometimes a challenging task because not always receiving surface water bodies are available in the neighboring. Consequently, the water treatment agencies often resort to infiltration pond facilities for discharging effluents from the treatment plant. This technical solution is considered extremely favorable because it recharges the groundwater bodies, increasing the availability and improving the qualitative status of the natural reservoirs. The daily operation of such infiltration pond facilities is often based on heuristic rules simply aimed at discharging the treated water volumes. Nevertheless, the functioning of these infrastructures strongly relies on some hydraulic and hydrogeological features of the hosting site. The knowledge of parameters such as the average vertical and horizontal hydraulic conductivity in the area surrounding the basins would allow for optimizing the water flows to the groundwater. This study compares some techniques for modeling clusters of interconnected infiltration ponds with the aim of estimating the average values of the hydrogeological parameters involved therein. The overall inverse model is based on a dynamical system derived from mass balance and Darcy's law. Within this general computational framework, several techniques have been implemented and tested, such as different Kalman filter versions. It is worth highlighting that the considered model is intrinsically ill-conditioned, and the right-hand side of the ODEs system is discontinuous: these issues somehow affect the accuracy of the tested techniques. This study has been conducted on synthetic data, partially based on the results of a previous study.

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Energy Transition Focused Abstracts:

MS07 / 769

Four-phase equilibrium calculation algorithm for water/hydrocarbon mixtures

Authors: Martin Jex[1]; Abbas Firoozabadi[2]; Mikyška Jiří[1]

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Successful large-scale compositional reservoir simulation requires robust and efficient equilibrium calculations. In recent years a large number of papers have been published on the topic of three-phase vapor-liquid-aqueous (VLA) equilibria
which frequently appear in hydrocarbon reservoirs. The presence of the aqueous phase increases the probability of equilibrium calculations to have issues. One may experience convergence problems or even not being able to distinguish a fourth phase altogether. This is generally due to the lack of good initial guesses, which is usually solved by proposing supplementary inital guesses which are designed to deal with a particular mixture. The commonly used approach is to perfrom a stability

test, before the equilibrium calculation,
which determines whether it is needed to add an additional phase. Another
benefit of this approach is that the result from the stability testing provides a good initial guess for the phase equilibrium calculation. In this contribution we derive a robust algorithm which can deal with up to four phase equilibrium
calculation. We demonstrate the algorithm and its robustness and efficiency
in several examples from literature (mainly computing the phase envelopes of
water/hydrocarbon mixtures).

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Energy Transition Focused Abstracts:

Poster / 771

Colloidosome-Transported Chemical Carbonate Precipitation (CTCCP): A Novel, Low-Emission Grouting Strategy for Cracks and Porous Media

Author: Jack Roden[1]

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Corresponding Author: jack.roden@strath.ac.uk

As the world continues to develop in a worsening climate crisis, greener alternatives to cement-based grouting must be implemented. Biological calcium carbonate precipitation methods such as Microbially Induced Carbonate Precipitation (MICP) show promise as alternative grouting strategies, but their biological nature lends itself to issues concerning environmental sensitivity and limited CaCO3 yield. This research aims to remedy that by developing a novel carbonate-based grouting strategy based entirely on inanimate physicochemical processes.

CTCCP utilises "dry solution"colloidosome technology to allow for the controlled delay of simple CaCO3-precipitating reactions for use in ground stabilisation. The reagent solutions are emulsified in the air using hydrophobic fumed silica, forming micro-scale colloidosomes that take the form of a dry powder. These powders can then be mixed thoroughly without any contact between the reagents, delaying the reaction. Once transported via a suitable carrier fluid to the area designated for grouting, the colloidosomes can then be released by initiating a reaction which disables the hydrophobic surface treatment of the colloidosomes. The reagents are then free to react and precipitate CaCO3, grouting the target area.

At this early proof-of-concept stage, we have shown that colloidosomes can be synthesised *via* standard and novel synthetic processes, the latter of which may help with optimising the technology. We have also shown that a range of water-soluble, CaCO3-precipitating reagents can be encapsulated at a variety of concentrations, and that the colloidosomes can be released by both mechanical force and chemical reaction.

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Energy Transition Focused Abstracts:

Poster / **772**

Experimental studies of slow drainage in porous media: Effect of the randomness of the porous medium on the fluid flow

Author: Khobaib Khobaib[1]

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Two Phase flows are used in several fundamental and practical applications. For many applications, it is crucial to understand the physics of multiphase flow under the effect of the capillary, gravitational, and viscous fields 1. Here, I will demonstrate experimentally how pore disorder affects fluid displacement. I am investigating the drainage of the liquid in porous media and studying the influence of the randomness of the 3D-printed porous medium structure on the fluid front. My experimental setup allows us to control the gravitational field precisely, and I can thus study the relative effect of the hydrostatic pressure field and the capillary fluctuation. This work offers a better understanding of the impact of the pore-scale disorder on flow behaviors in the porous medium.

Participation:

In-Person

References:

Vincent-Dospital T, Moura M, Toussaint R, Måløy KJ. Stable and unstable capillary fingering in porous media with a gradient in grain size. Communications Physics. 2022;5(1):306.

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Energy Transition Focused Abstracts:

Poster / 773

An energy stable SPH method for fluid-solid coupling in geological porous medium

Authors: XINGYU ZHU[None]; Xiuping Wang[None]

Co-author: Shuyu Sun [1]

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The great challenge for understanding the porous media is the heterogeneity in rocks known as the core structures with different types and scales. Recently, with the development of digital core technology, more reliable information can be used to indicate the potential influence of fluid flowing in porous media. Thus, the pore-scale modeling that simulates the fluids flow directly in the three-dimensional Micro-Nano core structures provides a more accurate and stable prediction of the flowing. However, traditional numerical methods suffer a number of difficulties in pore-scale modeling, especially when the pore structures are complex, known as a type of fluid-solid coupling. This paper adopts a modified particle-based method, Smoothed particle hydrodynamics (SPH), to pore-scale modeling to improve the stability and accuracy of the incompressible fluid flow within complex geometry. The novel method divides the domain into system and surroundings, represented by fluid and solid particles, respectively, where the interaction between the fluid and solid particles can be simulated naturally without additional coefficients. The governing equations for the different particles are consistent, and constraints are adopted to restrict the motion of solid particles and the incompressibility of the fluid. We design numerical schemes based on the projection method to preserve the unconditional energy stability, indicating unconditional numerical stability, which allows a large size of the time step and accurate fluid-solid coupling. The feasibility and novelty of the proposed method are verified by comparing it with the experimental benchmark. Furthermore, our method has great potential for the problems of grain flow.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS01 / 774

A micro-scale study of CO2 mobility control characteristics of a green foam in porous media

Author: Tongke Zhou[1]

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Geological carbon dioxide (CO2) sequestration is considered as a technology for reducing the atmospheric content of CO2 [1, 2]. CO2 has been widely injected into saline aquifers or oil reservoirs for sequestration in recent decades [3]. This process involves displacing resident fluids from porous media, which is unstable due to the unfavorable mobility ratio between the resident and injected fluids. Although some fluids with chemical agents are used to inhibit gas channeling, these methods tend to cause pollution and damage to environment and formation.
In this work, we propose an environmentally friendly aqueous foam to control the CO2 mobility and enlarge its sweeping efficiency. To get insight into the CO2 mobility control behavior of the aqueous foam, we conducted a series of analysis including the stabilization and rheological properties of the CO2 foam with cellulose nanofibrils (CNFs) and camellia oleifera saponin (COS). Pore-scale dynamics of CO2 foam in a 2D visual micromodel obtained from a real core via micro-CT images were analyzed. The stabilization and rheology experiments allowed us to explore the special properties of foam as a CO2 carrier in porous media, while the microfluidic experiment was used to evaluate the dynamics of generation and rupture of foam bubbles with enhancers. The microscopic visual experiments make it possible to analyze the flow behaviors and sweep efficiency increase of foams in porous media simulating aquifers and oil reservoirs.
Results demonstrate that the higher viscoelasticity and stability cause large numbers of small bubbles to group together, providing greater flow resistance to control the mobility of CO2. CNF/COS foam carries CO2 deeper into porous media and increase CO2 saturation in aquifers and oil reservoirs, while also showing a higher oil resistance stability compared to bare surfactant foam. Abundant hydrogen bonds between CNFs and COS molecules support the formation of tight bubble film which can stably encapsulate CO2 and inhibit its diffusion. The interlacement and entanglement of CNFs endows liquid phase with high viscosity, which restrains liquid drainage and improves the interfacial viscoelasticity of the bubble film.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS10 / **775**

Scale-independent rock heterogeneity classifier applied to micro-tomography images

Authors: Ali Mohamed[1]; Masa Prodanovic[2]

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Typical geological systems are composed of a broad spectrum of porous media with regionalized rock properties such as porosity or permeability varying by orders of magnitude within a volume of study. Upscaling the petrophysical rock properties is controlled by the rock pore size and type heterogeneity which is a scale-dependent variable. At the same time, Recent advances in high-resolution imaging techniques have provided a wealth of 2D and 3D datasets that reveal the microstructure of rocks and soil on scales ranging from nanometers to centimeters. However, the images by themselves greatly vary based on imaging technique details and objectives of research taken in porous media. Automating the rock heterogeneity estimation regardless of the type of imaged input would be of great interest to geology and engineering communities.

We provide an automatic scale-independent method for classifying rock heterogeneity. Our method modifies local order metrics by (Torquato et al. 2022). They used synthetic, two-phase porous materials and compared relative ranking of disorder for materials with the same length scale and porosity. Our modification introduces length scale independence and was verified against three categories of benchmarks, all together 87 geologic and synthetic 3D CT datasets found in Digital Rocks Portal (https://www.digitalrocksportal.org/). Further, the method performs better compared to other geostatistical heterogeneity coefficients including Dykstra-Parsons, Lorenz, and pore heterogeneity coefficients. A sensitivity analysis has revealed a significantly faster performance and reliable true heterogeneity of the 3D version compared to the apparent heterogeneity seen when splitting 3D volume in its 2D cross-section. Thus, whenever possible, 3D datasets should be used in analysis of porous media. While our application is to the images in Digital Rocks Portal and we hope that will in future ease automated curation of images in the portal, the method should extend easily on any porous media imagery.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 776

Combining Molecular Dynamics and Machine Learning to determine CO2 adsorption features on amorphous nanosurfaces

Authors: Ivan Lunati[1]; Mattia Turchi[2]; Sandra Galmarini[2]

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In contrast to crystals, amorphous materials are characterized by a disordered structure that dictates adsorption at the surface. Understanding how amorphous features affect gas sorption is crucial to rationally design efficient amorphous adsorbents. Recently, we have demonstrated by Molecular Dynamics (MD) simulations the differences between the adsorption of CO_2 in crystalline (Fig 1a) and amorphous (Fig 1b) silica nanopores1. The heterogeneous features of the amorphous nanosurfaces (e.g., roughness, functional groups, hydroxyl groups, oxygen vacancies) enhance CO_2 adsorption with respect to analogous crystalline surfaces, making amorphous material interesting for many industrial application (including catalytic processes). Here, we propose to use machine learning to more faithfully characterize and describe CO_2 adsorption in amorphous nanopores.
First, we employ a segmentation algorithm to identified the irregular adsorption patterns; then, we use a classification algorithm to group similar patterns; and finally, we correlate the adsorption patterns with the underlying surface features. This framework can help identify the most efficient functional groups, paving the way to a computer-aided design of amorphous sorbents that can be employed in many industrially relevant processes. Typically, the region of influence of surface groups can be inferred by means of radial density functions that enable calculating the residence time of the CO_2 molecules within spherical neighborhoods that are defined around the surface sites of interest, which has been a-priori determined1. Although this approach allowed us to demonstrate the major contribution of oxygen vacancies, CO_2 adsorption patterns are very irregular (Fig 1b) and it is not trivial to correlate the high density regions to the underlying heterogeneous structure in the case of amorphous surfaces.
As an example, we consider the methanation reaction, which has been shown to be catalytically enhanced on amorphous silica nanospheres that are specifically engineered to exhibit a high density of surface defects[2].

Participation:

In-Person

References:

References
1 Mattia Turchi, Sandra Galmarini, and Ivan Lunati. "Amorphous matters: surface defects in nanopores enhance CO2 adsorption". In: to be submitted (2023).
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MS20 / **777**

Modeling contraction in linearly elastic tissue using point sources

Authors: Wietse Boon[1]; Fred Vermolen[2]

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We focus on the contractive forces exerted by fibroblast cells during dermal wound healing. To capture these effects, we construct and analyze two modeling approaches under the assumption of linearized elasticity. The first approach introduces a collection of point forces on the boundary of each fibroblast cell and uses a superimposition principle. The resulting partial differential equation is analyzed rigorously using a sum of radially weighted Sobolev spaces and we propose two discretization approaches. The first is a direct application of the finite element method, which is expected to suffer from sub-optimal convergence. Therefore, a second approach is proposed in which the known singularity is subtracted from the solution and a smooth correction field is sought.

The second modeling approach employs an isotropic stress point source in the cell center. By identifying this model as a limiting case of the point force model, we analyze the model using appropriately weighted Sobolev spaces. By identifying the behavior of the solution, the singularity removal method is shown to be applicable here as well. Moreover, we show that the introduction of the solid pressure leads to a locking-free discretization method using familiar Stokes-compatible finite elements.

The validity of both modeling approaches is confirmed by numerical experiments in two and three dimensions. Moreover, we demonstrate that the rates of convergence of the numerical methods agree with those predicted by the theory.

Participation:

In-Person

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778

Machine learning augmented permeability prediction from X-ray micro-computed tomography reservoir rock images

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The petrophysical properties are crucial to understanding the fluid (oil, gas & water) flowing through the reservoir. Due to the complex nature of petroleum reservoirs, the grain, pore, and throat properties are of utmost importance. Determining these properties with utmost care and precautions can lead to a better understanding of porous media and ultimately to enhanced recovery. The permeability calculation with pore characteristics has long been under discussion, and various equations have also been derived. We present a research study aimed at testing the predicting power of machine learning (ML) algorithms for permeability prediction by considering both the pore and throat properties. We prepare a training set containing 3D scans of Berea sandstone subsamples imaged with micro X-ray tomography and corresponding permeability values simulated with the Pore Network

Modelling (PNM) approach. The 3D image samples were used as input for model training and prediction. We compare the predictive power of various machine learning methods like gradient boosting (LightGBM, CatBoost, XGBoost), random forest (RF), and Decision tree (DT). We also obtained a porosity-permeability relationship that provides a better prediction of the permeability compared with predictions obtained by previous correlations. The results obtained using the machine learning developed in this study are in satisfactory agreement with the actual permeability of the porous media. The K-fold cross-validation algorithm (k-foldCV) is applied to optimize the hyper-parameters of the ML algorithms. Each machine learning technique has performed satisfactorily in terms of determination coefficient (R2), mean square error (MSE), root mean square percentage error (RMSPE), and computation time. The results demonstrate the applicability of machine learning techniques for image-based permeability prediction and open a new era of Digital Rock research.

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MS06-A / **779**

Competitive adsorption of CO_2 and CH_4 in functionalized amorphous-silica nanopores

Authors: Mattia Turchi[1]; Ivan Lunati[1]; Sandra Galmarini[None]

[1] *Empa*

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We investigate the mechanisms of competitive adsorption of CO_2 and CH_4 molecules in silica nanopores characterized by different physico-chemical features. We study the influence of different physical properties (e.g., surface roughness and the geometric arrangement of functional groups) and chemical heterogeneity (e.g., the number of hydroxyl, -OH, and ethoxyl, -OCH_2-CH_3, groups at the nanopore surface) on the affinity for CO_2 and CH_4, as well as on the resulting mobility. Notably, hydroxyl (Fig 1a) and ethoxyl (Fig 1b) are among the most common surface groups found on silica substrates that are synthesized from the Tetraethyl orthosilicate (TEOS) precursor. A recent work 1 showed the potential of hydrophilic (high density of -OH groups) and hydrophobic (high density of -OCH_2-CH_3) membranes for fluid separation. From the results of molecular dynamic (MD) simulations, we extract the most relevant parameters that describe the adsorption of the CO_2, CH_4, and mixtures of the two. We report the key findings of the atomistic investigation and discuss the relevant surface properties that need to be considered for a faithful upscaled description of the resulting macroscopic flow and of the adsorption of CO_2/CH_4 in nanoporous silica. In particular, we focus on the differences between the two functionalizations of the surface and their selectivity towards the two gases. The results of the MD simulations enable the rational design of amorphous adsorbents that can be tailored to adsorb the required ratio of CO_2 to CH_4 molecules. Precisely designed selective adsorbents can find application, for instance, in shifting the equilibrium of the methanation

reaction ($CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$), which is gaining attention in synthetic fuel production aiming at mitigating CO_2 emission.

Participation:

In-Person

References:

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780

Exploring the Potential of Pre-trained Backbones for Analyzing Raster Electron Microscopy Images of Opalinus Clay

Author: Marco Brysch[1]

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Understanding the microscopic pores in a potential host rock such as Opalinus clay is crucial for determining the physical properties of the material including permeability and strength, which are important for safe radioactive waste disposal. One method for visualizing and characterizing these pores is via scanning electron microscopy (SEM), which allows for high-resolution imaging at the nanoscale. However, the process of segmenting and analyzing SEM images for pore identification can be difficult due to limitations in resolution and the need for manual input. Recently, machine learning (ML) and deep learning (DL) techniques have been employed to develop automated methods for analyzing such images and segmenting pores providing faster and more consistent results that do not rely on user input.

Backbones are essential components in the field of DL, as they are able to learn features that are necessary for the identification of objects and hence for image processing. Objects are described by a specific set of features that makes them unique. Therefore, an important part of image processing is a comprehensive set of features. Pre-trained backbones, trained on datasets such as ImageNet that contains millions of everyday images, have a variety of features that are useful for image processing tasks. However, specialized applications such as automated analysis of microscope images often require features that differ from those of pre-trained backbones. In addition, the limited availability of microscope images may cause ML to outperform DL to some extent [Maitre et al., 2019]. This is because, in supervised machine learning, features are manually created before training, which requires careful feature selection by an expert. In this study, we investigate the training behavior of

pre-trained backbone models on new SEM images. The backbone models have been trained through two stages: a warm start and fine-tuning. During the warm start, only the object classification was trained while maintaining the features from the ImageNet dataset. In the fine-tuning stage, all layers were trained to adapt and learn new features from the SEM images. The fine-tuning process was used to observe the model's ability to adapt to the new data.

We examine eight different backbones, including VGG16, VGG19, ResNet50, Desenet, Xception, and Mobilenet. Our training data consists of 2000 SEM images showing both the background and pores of an Opalinus clay sample. To train a backbone with this relatively small amount of training data, we used a transfer learning technique. To get a general sense of the behavior of different DL backbones, we examined the gradient during the learning process using gradient-weighted class activation mapping (grad-CAM) [Selvaraju et al., 2019]. Through analysis of the model's adaptation efforts, we demonstrate which pre-trained backbone models demonstrate good training behavior on SEM images and provide an estimation of the amount of data needed for effective training.

Participation:

Online

References:

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781

A New Model of Shift Factor for Sphere Pack Samples by 3D Microscale Flow Simulation of Shear Thinning Fluids

Authors: Mehdi Amiri[None]; Jafar Qajar[None]; Ali Qaseminejad Raeini[1]; Amir Raoof[2]

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The study of non-Newtonian fluid flow through porous media is crucial for numerous applications, including heavy oil recovery, polymer-enhanced oil recovery, and liquid polymer molding 1. For the flow of non-Newtonian fluids at low velocities, an adapted version of Darcy's law is often used. Here, the constant viscosity is replaced by a variable viscosity that depends on the porous medium [2]. This viscosity is a function of shear rate, which in turn is dependent on a coefficient termed the "shift factor." The shift factor depends on the fluid and rock types.
Numerous models have been proposed for calculating the shift factor in sphere pack samples, where it is solely dependent on the power law index [3, 4]. However, given that the porosity, formation factor, and permeability in sphere pack samples can vary, the need to investigate the shift factor across different sphere pack models has attracted significant attention. In this study, we began by reconstructing sphere pack models with varying porosity, permeability, and formation factors. We

then simulated the flow of non-Newtonian fluids, each with a different power-law index, within these models.
Next, we evaluated the shift factor for each combination of fluid and rock properties. It was observed that the shift factor fluctuated with changes in porosity, permeability, and the formation factor. Finally, we examined the relationship between the shift factor and the rock properties, as well as the power-law index. The findings from this study can be invaluable for parameterizing models of polymer flow through porous media.
Keywords: Shift factor, Sphere pack samples, Microscale flow simulations, Shear-thinning fluid.

Participation:

Online

References:

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MS09 / 783

Volume of Fluid based study of the three phase dynamic contact line in the wetting of a thin channel.

Authors: Yash Kulkarni[1]; Tomas Fullana[2]; Stephane Zaleski[1]; Stephane Popinet[1]; Mathis Fricke[3]

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A continuum sharp-interface modelling of the molecular motion in the vicinity of the three-phase dynamic contact line is a significant research problem 1 having extensive practical relevance [2]. It is a prerequisite to full pore-scale Direct Numerical Simulation (DNS) with a high-fidelity representation of dynamic wetting phenomena. To investigate the three-phase dynamic contact line in the wetting of small pores, we numerically design a setup consisting of a pressure gradient-driven two-phase flow inside a thin channel (width ~ 0.1 - 10μm). The two phases are separated by an interfacial layer with surface tension, that meets the pore wall, hence, a three-phase dynamic contact line is formed. This setup is then studied numerically by solving the planar two-phase Navier-Stokes equations, comparing three contact-line boundary conditions: the Navier-slip boundary condition, the super-slip boundary condition and the generalized Navier boundary condition (GNBC). We use the

Basilisk flow solver to do Volume-of-Fluid (VOF) based simulations with the surface tension force computed using the Continuous-Surface-Force method and curvature calculations using the Height-Function method. Steady-state solutions are found for all three boundary conditions and a critical capillary number is predicted beyond which no steady-state solution exists. We thus extend previous contact line modelling using the VOF method [3],[4]. Similar to [3], we see that the Navier-slip model with a constant microscopic contact angle is weakly singular. This singularity does not prevent the prediction of the critical capillary number for wetting. The advantage of this new setup over the previous "hydrodynamic assist"setup of [2] and [3] and the "sheared droplet"setup of 1, is its direct relevance to the DNS at small pore size and the opportunity to reduce the range of scales involved. Due to the quadtree adaptive mesh refinement (AMR) and parallel-processing capabilities of our code, a parametric study with realistic nanometric slip length is possible and interesting flow features and scaling laws are discovered in the vicinity of the contact line.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-B / 785

Bubble Coarsening Kinetics in Porous Media

Authors: Yuehongjiang Yu[None]; Chuanxi Wang[1]; Yashar Mehmani[2]; Ke Xu[1]

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Bubbles in subsurface porous media spontaneously coarsen to reduce free energy. Bubble coarsening dramatically changes surface area and pore occupancy, which affect the hydraulic conductivity, mass and heat transfer coefficients, and chemical reactions. Coarsening kinetics in porous media is thus critical in modeling geologic CO2sequestration, hydrogen subsurface storage, hydrate reservoir recovery, and other relevant geophysical problems.

We show that bubble coarsening kinetics in porous media fundamentally deviates from classical Lifshitz-Slyozov-Wagner theory, because porous structure quantizes the space and decouple the mass transfer coefficient from the bubble size. We develop a new coarsening theory that agrees well with numerical simulations. We further identify a pseudo-equilibrium time proportional to the cubic of pore size. In a typical CO2 sequestration scenario, local equilibrium can be achieved in 1s for media consisting of sub-micron pores so local equilibrium can be presumed, while in decades for media consisting of 1 mm pores so capillary equilibrium fails.

This work provides new insights in modeling complex fluid behaviors in subsurface environment. In addition, along with our preceding works, we demonstrate that the porous media rescale mass transport of discrete fluid systems, by 1) modifying the free energy vs. volume correlation, and 2) decoupling the mass transfer kinetics from blob size.

Participation:

In-Person

References:

1Yu, Y., Wang, C., Liu, J., Mao, S., Mehmani, Y., & Xu, K. (2023). Bubble coarsening kinetics in porous media. Geophysical Research Letters, 50(1), e2022GL100757. https://doi.org/10.1029/2019gl085175
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https://www.pnas.org/doi/10.1073/pnas.2024069118

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Energy Transition Focused Abstracts:

Poster / 786

A numerical study on decreasing CO2 emission by flue gas injection into heavy oil reservoirs

Authors: Yashar Tavakkoli Osgouei[1]; Mehmet Onur Doğan[1]; Caglar Sinayuc[1]

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The production of heavy oil is challenging because of its higher viscosity and lower mobility. Although thermal-based methods are useful to cope with these problems through heat injection, the application of thermal recovery method are expensive and not always effective methods. Therefore, different alternatives were considered with respect to conditions of heavy oil reservoirs. Non-condensate gases like flue gas injection is widely used in heavy oil recovery. The flue gas includes approximately 80% N2 and 20% CO2 1 . The flue gas injection is an effective method for improving not only heavy oil recovery, but also environmental issues. The flue gas injection can increase recovery efficiency by gas expansion, viscosity reduction, and reservoir repressurization. In addition, the interaction of flue gas components with reservoir fluid under high temperature and pressure conditions of reservoir contributes to higher recovery factor of heavy oil [2]. Numerical study was carried out to investigate the effect of CO2 percentages of flue gas on oil production performance. The numerical results showed that reservoir pressure in higher CO2 percentage has experienced

larger decrease during flue gas injection. This can be attributed to higher solubility of CO2 than N2 in heavy oil at the same reservoir temperature. The presence of gas solution in heavy oil contributes to higher performance of oil production. The main reason for it can be viscosity reduction in heavy oil. In fact, the solution gas composition in the heavy oil provides a driving force for increasing heavy oil mobility in terms of the CO2 content [3]. The higher tendency of CO2 in flue gas to form miscibility with heavy oil components not only enhances heavy oil production performance, but also reduces CO2 emission by different industries as long as the injected CO2 is captured and recycled.

Fig. 1. Pressure distribution at injection (a) CO2 100% (b) CO2 20%-N2 80%

Fig. 2. Pressure drop in the reservoir

Fig. 3. Cumulative oil produced in production well

Participation:

In-Person

References:

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Poster / 787

Nuclear magnetic resonance of drainage and imbibition: Correlating structure and dynamics

Authors: Quirine Krol[1]; Matt Skuntz[2]; Isaak Thornton[3]; James Wilking[1]; Evan Schehrer[1]; Sarah Codd[None]; Joseph Seymour[1]

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Drainage, imbibition and steady state two phase flow in porous media have an abundance of applications in physics, chemistry and engineering. Experimental methods to capture this phenomena are

often limited to two dimensional setups, refractive index matching and/or are too slow to capture the dynamics at a resolution relevant to the physics at the pore scale. We utilize nuclear magnetic resonance methods to retrieve 1D spin-echo intensity and phase-angle profiles with a temporal and spatial resolution of 20 ms and 70 microns respectively. We compare first and secondary imbibition, drainage and steady state two-phase flow of a wide variety of three dimensional microstructures ranging from bead-packs, sticky hard spheres and 3D printed heterogeneous porous media. The latter is used to include both model media based on Gaussian random fields and complex microstructures based on micro-computed tomography data of snow. We extend analysis of standard 1D spatial profiles used to determine water saturation, to measure velocity and correlate signal attenuation to local velocity fluctuations. With this study we demonstrate that size and duration of local surges can be related to the heterogeneity of the porous media and has future potential to measure effective dispersion coefficients in steady state two-phase phase flow.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS09 / 788

Discrete Element Method modelling of non-active clays

Author: Arianna Gea Pagano[1]

Co-authors: Vanessa Magnanimo [2]; Alessandro Tarantino [3]

[1] *University of Glasgow*

[2] *University of Twente*

[3] *University of Strathclyde*

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Soils are porous multiphase geomaterials, composed of i) a particulate solid phase, and ii) a fluid phase, hosted within the soil's porosity. Due to their complex discrete nature, the macroscopic response of soils depends on the mechanisms occurring at the particle or pore scale. The particle-to-particle interactions can be mechanical and/or electrochemical in nature, depending on the soil mineralogy and particle size distribution. These interactions affect particle arrangements and kinematics, and the evolution of the soil's fabric and pore size distribution upon loading. Understanding the mechanisms occurring at the particle or pore scale is crucial to the prediction of soil macroscopic responses under different loading conditions, where these cannot be easily reproduced using the framework of continuum mechanics.
Exploring the particle-scale mechanisms and their evolution upon loading in a direct experimental fashion is extremely challenging for fine-grained soils such as clays, due to the small (sub-micron) particle size. In the absence of particle-scale experimental evidence, a valuable alternative to explore the particle-scale behaviour is to perform "virtual"experiments, where soils are modelled as discrete particulate media using the Discrete Element Method (DEM). Here, we present an overview of the capabilities of a DEM numerical framework specifically formulated to simulate non-active clays. The inter-particle interactions implemented in the force-separation laws of the DEM model

(electrochemical and mechanical interactions) are able to reflect the effect of the chemistry (pH and dielectric permittivity) of the fluid filling up the pore space on the macroscopic behaviour. The DEM framework, informed by existing experimental evidence (1) and proved to capture several aspects of the one-dimensional compression of non-active clays in oedometric conditions ([2]), was challenged to reproduce the behaviour of clay upon simple shear. Particular focus was given to the effect of the initial loading-induced particle orientations and fabric on the shearing behaviour, and on the evolution of both the soil's "macroscopic"porosity (e.g. void ratio) and pore-size distribution upon loading. The results of this study allowed to shed light on peculiar small (particle or pore) -scale mechanisms leading to the macroscopic observations upon which the continuum constitutive models used in conventional geotechnical engineering applications are formulated.

Participation:

In-Person

References:

1 Pedrotti and Tarantino, 2017. An experimental investigation into the micromechanics of non-active clays. Géotechnique 68, No. 8, 666–683, https://doi.org/10.1680/jgeot.16.P.245
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Energy Transition Focused Abstracts:

Poster / 790

Functional design of porous systems by systematic patterning of flat knits

Author: Leon Pauly[None]

Co-authors: Lukas Maier ; Ulrich Nieken [1]; Götz T. Gresser [2]

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[2] *DITF Denkendorf, ITFT University of Stuttgart*

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The porous properties highly determine the physical properties of materials like density, stiffness and flow transport properties. This poster wants to contribute to the question whether knitted pore systems can be designed and optimized for highly functional garments like sportswear or be used as functional carriers in technical products or processes. In a new combined wicking and drying experiment, textile fabrics are investigated concerning their transport properties. The vision of this work is, that understanding of the porous properties of knitted fabrics by systematically changing the geometrical properties only by patterning deepens the understanding of the porous system and its transport characteristics
Textiles can be interpreted as porous systems consisting of fibers arranged in repeating patterns. 1 In combination of different materials and textile production processes the structure of textile porous systems can be altered in a huge range. Pores in textiles can be systematically described on the scales fiber, yarn and fabric. Micropores occur on the fiber scale, Mesopores occur on the yarn scale and

macropores on the fabric scale respectively. [2] For knitted fabrics, especially macropores with pore sizes of 100 µm and higher can be systematically altered by the patterning in the knitting process. This poster focusses on non-standard porous patterns which are designed to have different amounts of pores on the meso- and macroscale. Previous work in this field is is focussed on standard patterns like single jersey, double jersey and rib patterns (e.g. [3]) and considers only porosity as porous property Therefore, we introduce an extended model for knitted fabrics which is parametrized with the yarn characteristics and the patterning and gives effective parameters like pore size distribution, fabric density and thickness. For experimental validation, different patterns which gradually differ in meso- and macropore distributions are knitted on an automated flatknitting machine and analyzed via automated imaging. The porous fabric properties are then correlated with the results from the new combined wicking-drying experiment.
The new experiment is presented and its results can be transferred to other fabric technologies. The poster should give an inspiration for function driven design by the concept of textiles as porous media. The geometrical parameter space and the relation to effective mass transport properties can initiate and accelerate development processes with knitted fabrics in a broad field of applications like tissue engineering.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / **795**

Fracture permeability evolution as a result of geochemical granite alteration in geothermal systems

Authors: Nick Harpers[1]; Jim Buckman[1]; Hannah Menke[1]; Julien Maes[1]; Niko Kampman[2]; Andreas Busch[1]

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Geothermal systems in crystalline basement rocks require fractures and faults to allow economic heat production. Sufficient permeability of these flow paths is vital and affects the lifetime of such systems. As fluids are produced and reinjected, the resulting flow, fluid mixing as well as related

pressure and temperature changes affect the geochemical equilibria between fluids and host rock. Disequilibria of fluids and rock then potentially drive dissolution, precipitation, or other geochemical alteration processes (e.g., illitisation). Such changes can change then mineralogical and geometrical properties of fractures, resulting in hydraulic property changes of the major flow paths of the fault zones. Cornwall in SW England hosts several granitic plutons that are the subject of current geothermal projects (United Downs Deep Geothermal Power and Eden Projects). These projects target fault zones in crystalline rock that provide pre-existing pathways for fluid flow.

To study the effects of geochemical alterations on fracture permeability in granites, we conducted a series of long-term reactive transport experiments in our unique flow-through reactor setup. Carnmenellis granite samples from central Cornwall have been collected of which small plugs (15 mm length, 10 mm width) and powders (< 125 μm grain size) were prepared. A tensile fracture was induced into the plugs to allow flow along the samples. We injected water with different fluid composition, representing different diluted to heavy brines encountered around geothermal systems, into the fractured granite plugs and pulverized gouges at 80 ℃ and 20 MPa confining pressure. The development of fracture and gouge permeability as well as effluent composition are analysed. CT-scans before, in-between, and after experiments are used to analyse changes in fracture and gouge structure. To complement the experiments, we model our system with GeoChemFoam [Maes and Menke, 2021], a reactive-transport modelling code that combines flow and transport calculations from OpenFOAM with geochemical calculations. The CT-scans of our samples act as basis for mesh and mineral distribution.

Participation:

In-Person

References:

Maes, J., and H. P. Menke (2021), GeoChemFoam: Direct Modelling of Multiphase Reactive Transport in Real Pore Geometries with Equilibrium Reactions, Transp. Porous Media, 139(2), 271-299, doi:10.1007/s11242-021-01661-8.

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MS09 / 796

CFD simulation of particle capture in open-cell foams: filtration efficiency and comparison with granular beds

Author: Enrico Agostini[1]

Co-authors: Marion Servel [2]; Yacine Haroun [2]; Maxime Moreaud [2]; Frederic Augier [2]; Gianluca Boccardo [3]; Daniele Marchisio [3]

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The problem of filtration for flows carrying particulate matter is of interest in many different fields: both for drinking water purification, in biological sterilization processes, or in the chemical and process industry for the removal of solid particulate feed of catalytic packed-bed reactors in refining processes.
Traditional filters show inefficiencies in removing particles with dimensions in the range 1 < dp < 20 μm, or induce too high a pressure drop, due to solid build-up in the filter leading to exponentially increasing pressure drops. The deposition phenomena of such systems are analogous to those described by Yao et al. (1971) for water filtration in granular beds. When the solid density is much higher than the liquid one, the captation is mainly the result of inertial deposition and steric interception with the solid collector.
One potential solution is the use of innovative open-cell ceramic foam structures as filtering media. Their open cellular structure makes them suitable for deep-bed filtration and moreover their high porosity and specific surface results in lower pressure drops compared to other packing media, such as granular beds. However, the influence of their geometrical structure and topology on the characteristic length and filtration efficiency remains an open problem.
The aim of this work is to investigate fluid flow and particles capture inside ceramics foams, to extract the key parameters and characteristic lengths affecting the filtration efficiency and compare them with more classical granular beds. The investigation is carried out performing numerical CFD simulations of the fluid flow inside foams geometries obtained either from x-ray tomography reconstruction or from digital generated model using an improved workflow based on Agostini et al. (2022), allowing the exploration of a large set of parameters, and able to reproduce both the geometrical structure and the macroscopic behaviour of experimentally investigated solid foam structures.The carried solid particles are represented by Lagrangian Discrete Particle Model (DPM) simulations, under the hypothesis of laminar regime and diluted systems and no influence of the particle on the fluid flow.

Participation:

In-Person

References:

Yao, K.M., Habibian, M.T., O'Melia, C.R., 1971. Water and wastewater filtration. concepts and applications. Environmental science & technology 5, 1105–1112. Agostini, E., Boccardo, G. and Marchisio, D., 2022, "An open-source workflow for open-cell foams modelling: geometry generation and CFD simulations for momentum and mass transport.", Chemical Engineering Science: 117583.

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Energy Transition Focused Abstracts:

MS06-A / 797

Dewatering and consolidation of clay slurries

Authors: Ismail Myouri[None]; Angela Casarella[None]; Leo Pel[1]; Claire Chassagne[2]

[1] *Eindhoven University of Technology*

[2] *TU Delft*

Corresponding Authors: i.myouri@tudelft.nl, c.chassagne@tudelft.nl, l.pel@tue.nl, angela.casarella@3sr-grenoble.fr

Dewatering, which is the process of separating (colloidal) suspended particles from a solvent (usually water), is used in many engineering applications (sanitary engineering, dredging engineering…). Key questions associated with dewatering in the context of the reuse of dredged sediment are (1) what is the process kinetics, (2) how can these processes be optimized and (3) can the dewatered sludge be reused and for which application?
Dewatering and consolidation are functions of the suspended particles'size and type, and their solvent-mediated interaction. In this presentation, some examples will be given about the dewatering of suspensions and slurries as found in engineering applications 1. The presentation will focus on the behaviour of mineral clay suspensions (kaolinite, montmorillonite, illite) composed of particles of different particle sizes [2-5]. We will show that, depending on the particle size distribution and solvent properties, the system is either undergoing a slow sedimentation dominated by thermodynamic forces or a rapid sedimentation dominated by gravity. The sedimentation is followed in time using NMR and inferential image analysis, and the particles are characterized by size, density and electrokinetic charge. We show that the time evolution of the sedimentation behaviour can be modelled using an advection-diffusion equation. The advective term is a function of gravity, whereas the diffusion term represents either a hard-sphere repulsion or an effective stress, depending on whether thermodynamic forces dominate the system [6-8].
For a mixture of different clays, the settling and consolidation behaviour is shown to be significantly affected by the type of colloidal particles in the system, even in a small amount. For instance, the settling of a kaolinite and montmorillonite suspension with a kaolinite to montmorillonite ratio of less than 0.1 (in weight) will be dominated by the strong electrostatic repulsive forces generated by the montmorillonite particles.
These interactions are not yet implemented in traditional civil engineering consolidation models based on effective stress concepts. Nonetheless, as we will discuss, their presence dramatically affects the answers to the questions (1-3) cited above.

Participation:

In-Person

References:

1 Shakeel, A., Safar, Z., Ibanez, M., van Paassen, L., & Chassagne, C. (2020). Flocculation of clay suspensions by anionic and cationic polyelectrolytes: A systematic analysis. Minerals, 10(11), 999.
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Poster / 799

Numerical investigation of impacts of surface wettability on gas hydrate formation in porous media

Authors: Qian Zhang[1]; Dong Yanhui[1]; Deng Hang[2]; Wang Liheng[1]

[1] *Institute of Geology and Geophysics, Chinese Academy of Sciences*

[2] *Peking university*

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Gas hydrates are nonstoichiometric crystalline compounds consisting of water and gas molecules, and can play a pivotal role in sustainable development. The formation process of gas hydrates, including nucleation and growth, is intrinsically affected by mineral surfaces and pore confinement in geological sediments. But the mechanisms underlying hydrate formation in confined spaces are not fully understood because of heterogeneities in sediment properties, such as surface wettability. Many studies have indicated that a hydrophobic surface can promote gas hydrate formation through the tetrahedral ordering of the water structure and increased gas density at solid–gas-water interfaces, whereas hydrophilic surfaces exert the opposite effect. However, the combined effects of wettability on both multiphase flow and the formation of hydrates are rarely addressed. In this work, wettability-dependent CO2-water distributions and the corresponding CO2 hydrate growth were investigated using pore-scale modeling. Simulation scenarios with various water contact angles and gas injection velocities were enabled by coupling the two-phase flow solver in OpenFOAM and the geochemical modeling capability of CrunchFlow. Simulation results show that the heterogeneity of water distribution markedly increases as the water contact angle becomes larger after CO2 displacement. Water forms thin films when attached to hydrophilic surfaces but remains as droplets on hydrophobic solids. Compared to hydrophilic systems, the gas–water interface area in hydrophobic ones is larger owing to gas bubbles dispersed in water, which can promote CO2 dissolution and diffusion into the water phase. In the subsequent formation process of gas hydrate, the amount of hydrate growth is controlled by how fast the hydrate initially forms, which is largely driven by initial conditions and nucleation dynamics, as well as how rapidly the growth rate is reduced, which is controlled by the feedback between hydrate formation and diffusion limitation. Overall, this study demonstrates that surface wettability can play an important role in the gas hydrate formation process in porous media by affecting the gas–water distribution, gas diffusion behavior, and final gas hydrate saturation. These insights provide a more in-depth understanding of gas hydrate formation in porous media.

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Energy Transition Focused Abstracts:

801

Calculation method and numerical simulation of fluid phase behavior migration in nano-confined space of shale oil reservoir

Author: Renyi Cao[1]

Co-authors: Yuanzheng Wang [2]; Jinchong Zhou [1]; Zhihao Jia [1]; Linsong Cheng [1]; Hongxin Guo [1]; Yongchao Xue [1]; Pin Jia [3]

[1] *School of Petroleum Engineering, China University of Petroleum, Beijing*

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Daqing Gulong shale oil reservoir in China has developed nanopores, and the occurrence state and flow characteristics of oil are complex. In nanopores, due to the influence of nano-confined effect, the fluid phase behavior changes, which affects the initial fluid distribution in nanopore media. At present, the nano-confined effect and fluid phase behavior characteristics in different nanopore spaces are not clear. In this paper, the nano-confined effect and the initial occurrence state of fluid in different nanopore spaces of shale reservoirs are studied by theoretical calculation and numerical simulation.

In this paper, based on the contrast state law, the calculation formula of the critical parameter offset of nanopores is derived. Then, based on the state equation, the critical parameter offset is considered, and the capillary force and the molar volume reduction due to adsorption in nanopores are corrected. The modified gas-liquid equilibrium calculation method is formed, and a fluid phase behavior calculation correction method under the influence of nano-confined is established. Based on the pore distribution and fluid composition of Gulong shale oil reservoir, the phase envelopes of fluid in different pore radii of 3-50 nm are calculated and plotted. The phase behavior migration of fluid in different nanopores of shale reservoir is quantitatively calculated, and the phase behavior distribution of fluid in different scale nanopore media is clarified.

The results show that for the migration of critical parameters in nanopores, the smaller the pores, the more the heavy hydrocarbons, the more the migration of critical temperature and pressure. As the nanopore size decreases, the critical temperature and critical pressure become smaller and smaller, and the phase envelope range of the fluid becomes narrower and narrower. According to the original formation temperature and pressure of Gulong shale reservoir, the initial occurrence state of fluid in different nano-pore media under nano-confined conditions of Gulong shale reservoir is clarified: it is condensate gas phase in pore space less than 3nm, near condensate gas phase in pore space of 3nm-5nm, and volatile oil phase in pore space of 5nm-50nm.

In this paper, based on the contrast state law and state equation, a mathematical model for calculating the critical parameter migration of nanopores in shale reservoirs is derived and established by combining theoretical calculation and numerical simulation. The critical parameter migration of different pore spaces under the influence of nano-confined effect is quantitatively calculated. Taking the Gulong shale oil reservoir as an example, the fluid phase envelopes in different nanopore spaces are calculated and plotted, and the initial phase behavior distribution characteristics of fluid in different nanopore media of shale reservoirs are clarified, which provides theoretical reference value for the study of fluid initiation mechanism and efficient development of shale reservoirs.

Keywords:
Shale oil reservoir
Nano-confined
Phase behavior migration
Occurrence state
Numerical simulation

Participation:

Online

References:

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MS06-A / 802

Bridging the continuum and discrete models developed to simulate solute transport and distribution in drying porous media

Author: Abdolreza Kharaghani[None]

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Solute migration and formation of solids in capillary porous media exposed to evaporation is central to many engineering and environmental applications. In order to predict the evolution of solute concentration in a porous medium, the macroscopic continuum models (CMs) are commonly employed. However, the predictive aptitudes of the CMs is still questionable at this stage. In this work, we solve the classical advection-diffusion equation for solute transport in a capillary porous medium exposed to evaporation for the limiting condition of capillary-dominated regime. The solution of the CM is compared with pore network simulations. The results of both models are analyzed in terms of instantaneous and time-averaged local solute concentration profiles. On this basis, the ability of the CM to predict the time for the onset of solid formation (i.e. the time that is required for local solute concentration to reach saturation concentration) is assessed. Furthermore, we characterize the degree of heterogeneity in the liquid phase structure (i.e. splitting the bulk liquid into the main cluster, the isolated clusters and the isolated single menisci) by performing pore network Monte-Carlo simulations. Based on the statistical analysis of Monte-Carlo simulations, we compute the probability of first solids to appear in the respective liquid phase elements. Solute enrichment is more pronounced in the isolated single menisci and isolated clusters due lack or significant hindrance to back-diffusion as a result of discontinuity in the liquid phase.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS19 / **803**

Revealing multi-component 4-D heterogeneity in electrochemical systems via simultaneous neutron and X-ray tomography

Author: Pranay Shrestha[1]

Co-authors: Jacob M. LaManna [2]; Kieran F. Fahy [1]; Pascal Kim [1]; ChungHyuk Lee [3]; Jason K. Lee [1]; Elias Baltic [2]; Daniel S. Hussey [2]; David L. Jacobson [2]; Aimy Bazylak [1]

[1] *University of Toronto*

[2] *National Institute of Standards and Technology*

[3] *Toronto Metropolitan University*

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Simultaneous neutron and X-ray tomography (NeXT) harnesses the benefits of both X-rays and neutrons to enable truly correlative and high-contrast imaging of a wide range of multi-material systems. NeXT is especially well-suited to study fluid flow and morphological characteristics in porous media, such as porous layers found in electrochemical devices. In this study, we utilize *operando* NeXT to quantitatively reveal heterogeneity in morphology and liquid water distribution within fuel cell components. A novel interfacial tracking technique is used to characterize 4-dimensional (4-D, 3 spatial dimensions and time) morphology of cell components. Accurate tracking of interfaces enables us to define component boundaries in 4-D and analyze liquid water distributions within individual components during fuel cell operation. Heterogeneity in the morphology and liquid water distribution of fuel cell components, particularly within the central membrane, is found to depend upon location with respect to other cell components and operating conditions of the cell. Heterogeneous distribution of porosity within the cell is found to affect liquid water accumulation and consequently the hydration and mechanical properties of the membrane. With this study, we demonstrate how NeXT is a viable and powerful tool in quantitatively characterizing *operando* processes in multi-component electrochemical systems. The methodology presented here is more broadly applicable to diverse static, evolving, and *operando* systems.

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In-Person

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MS15 / **804**

Modeling time-dependent battery discharge rate using an autoregressive multiscale neural network

Author: Agnese Marcato[1]

Co-authors: Gianluca Boccardo [2]; Javier E. Santos [3]; Alejandro A. Franco [4]; Daniele Marchisio [2]; Chaoyue Liu [4]

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[3] *Los Alamos National Laboratory*

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Investigating the operation dynamics of energy storage systems, like lithium-ion batteries, is becoming increasingly important in a range of applications, from automotive to grid-connected energy storage. To simulate battery discharge we performed finite element simulations in unstructured grids. The transient simulations are focused on the cathode of the battery (i.e.: half-cell simulations), and the discharge at different C rates is explored 1. The mass and charge equations of balance are solved at the microscale on three-dimensional reproductions of cathodes geometries. Three phases are considered in the electrochemical model: active material, carbon binder domain, and electrolyte. The creation of the cathode geometries is based on the fabrication process of the electrodes which allows us to produce a wide range of geometries to perform numerical simulations on. Different amounts of active material at different degrees of compression (calendering) of the electrodes have been explored to create electrodes geometries that produce different battery discharge profiles. The results of these simulations are then interpolated back to a regular 3D grid. This whole process is very costly and cannot be integrated into optimization workflows.
The multi scale neural network (MSNet) has been employed to train data-driven models to perform different tasks related to transport in porous media. Notable examples include prediction of flow fields [2], electric potential [3], and concentration fields in reactive flows [4]. In all these applications, the target of interest is the steady-state solution of the field. Nevertheless, in the case of electrochemical transport in lithium-ion batteries we are interested in knowing the discharge profile in time at different rates. Hence, the data-driven model requires modifications to learn to model the temporal dynamics.
In this work we trained an autoregressive MSNet on a dataset of time-dependent 3D simulations of electrochemical transport in lithium-ion batteries. The network takes as input the geometrical descriptors and the operating conditions, together with a temporal feature, which is: the initial condition for the prediction of the first time-frame, or the previous time-frame prediction for the prediction of the following one. Using this approach, the transient nature of the dataset is preserved, since MSNet is provided with the complete ordered samples (from initial conditions to final time) at each epoch and learns how to dampen the prediction errors along the time-frames. The predicted fields are integrated in order to reproduce the discharge curves of lithium-ion batteries. The performance of the trained network is tested on new cathodes to show its generalization capabilities. We envision this work as a proof-of-concept of the feasibility of this approach leading to the employment of the autoregressive MSNet in optimization frameworks on a wider and more challenging datasets.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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MS02 / **805**

Functional Biochar for Contaminant Removal from Water

Authors: Haiyan Zhang[None]; Guoting Li[1]; Tannaz Pak [2]

[1] *North China University of Water Resources and Electric Power*

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Deterioration of water quality has become a critical global challenge. Commonly contamination of groundwater is caused by human activities at the surface including petroleum leakage from fuel stations, leakage of substances used and produced within manufacturing and chemical industries, and also importantly substances used in the farming industry 1. The contaminants of significance include a vast array of chemicals such as polyfluoroalkyl substances, fertilizers, pesticides, and antibiotics. Investing in new technologies to improve the quality of water resources is the key to resilience in a changing world.

Biochar is a stable and porous carbon-rich adsorbent material that is used to remove contaminants from water [2]. Biochar is produced through the pyrolysis process using relatively inexpensive and sustainable material (biomass) as feedstock. The performance of biochar depends on the biomass properties and the parameters of the pyrolysis process (such as pyrolysis temperature and heating rate). Pristine biochar with low surface functionality and small pore sizes offers limited adsorption capacity. A key consideration in improving biochar adsorption efficiency is to choose suitable biomass and activation of biochar [3,4]. Chemical activation is commonly used in which chemicals (e.g., acid or alkali, metal oxide or metal salt) are used to activate biochar.

Here we focus on contaminants introduced to the environment as a result of processes used within the farming and textile industries. Methylene blue (MB) is a dye which causes contamination in textile industry wastewater streams. Nitrate (NO3-) is a major contaminant that is caused by excessive use of fertilizers in the farming industry. MB removal from water has been researched significantly, in particular, sorbents such as activated carbon and biomass have been studied extensively. NO3- removal is more challenging, therefore, in most cases nitrate levels in water are reduced through dilution rather that removal. Here we report on the efficiency of clay-biochar composites for removal of NO3- and MB.

`Synthesis of functional clay biochar offers an economical method to remove contaminants from water [`

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS09 / 806

Pore network modeling of calcination in single particles with evolving microstructure

Authors: Xiang Lu[None]; Abdolreza Kharaghani[1]

[1] *Otto von Guericke University*

Corresponding Authors: abdolreza.kharaghani@ovgu.de, xiang.lu@ovgu.de

A pore network model for calcination of a single particle (made of magnesium carbonate) is developed in order to better understand and quantify the heat and mass transfer within the particle, morphological changes of its pore structure, chemical reactions and the connection to the particle' s fluid-solid surrounding. Both the pore space and solid skeleton of the particle are approximated as regular-lattice networks. Local reaction rates are expressed by the one-step kinetic model using the classical Arrhenius equation with constant coefficients. Mass balance equations are set up to solid elements (i.e. magnesium carbonate and magnesium oxide) and carbon dioxide at pores. At each time step, the size of solid elements and complementary pore structures is updated. Using this pore network model, the development of the carbon dioxide profiles at the surface as well as at the reaction front where the decomposition reaction takes place are predicted over time. Though this model is oversimplified from point of view of physics and chemistry, it shall serve as an essential step to develop superior pore network models that can simulate calcination of a single particle at reaslistic process conditions.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 807

Discrete fluid model for drying of capillary porous media with evolving microstructure

Authors: jing chen[None]; Xiang Lu[None]; Evangelos Tsotsas[None]; Abdolreza Kharaghani[1]

[1] *Otto von Guericke University*

Corresponding Authors: abdolreza.kharaghani@ovgu.de, jing.chen@ovgu.de, evangelos.tsotsas@ovgu.de, xiang.lu@ovgu.de

The microstructure of capillary porous media partially saturated with liquid water often changes in the course of drying. This significantly affects the structural and transport properties of porous media. In this work, a discrete pore network model has been developed that allows to describe the microstructure dynamics and mass transport kinetics of a model capillary porous medium under slow drying conditions. In the pore network model, the space occupied by the fluid phases is approximated by a three-dimensional lattice of interconnected spherical pores and cylindrical throats. Assuming laminar axial flow through each pore and throat, equations based on Fick's law and Poiseuille's law are solved to obtain the local fluid pressures and flow rates. Since the solid matrix of the medium slightly moves during drying, due to stress induced by capillary forces, the complementary pore network is updated over time and the pore/throat saturations are mapped to the new pore network in a physical way. The evolution of the microstructure and phase distribution over time as well as drying rate and time are simulated using this adaptive pore network model and compared to those predicted by a pore network model where the solid phase remains stationary during drying (see Fig. 1).

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 808

How does electrical field affects and enhances contaminant migration in porous media ?

Authors: Noura Eddaoui[1]; Cyprien Soulaine[2]

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In this work, we discuss the effects of the electrical field on the mobilization and the transportation of contaminants through porous media. In this type of process, various interactive electro-physico-chemical phenomena can occur, which makes it difficult to capture all of the process contribution (complexity) in a model. Therefore, the already existing models do not attempt to simulate the behavior of the entire system. The present work can be considered as a preliminary study toward the integration of new complexities and proposes a conceptual and numerical model simulating contaminant migration coupled to the electrical properties of the porous medium (including the electrical double layer and the displacement of charges). Issues such as the control of contaminant mobility, the ability to achieve remediation (cleanup) objectives, and the estimation of treatment efficiency criteria, will be discussed as well.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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MS01 / 809

Calibration curve generation for the use of Xenon as a pressure indicator in porous media using micro computed tomography

Authors: Antje van der Net[1]; Maja Ruecker[2]; Mark Willemsz[2]

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[2] *Mechanical Engineering, Technical University Eindhoven, the Netherlands*

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Subsurface carbon-dioxide (CO_2) and hydrogen (H_2) storage are considered a promising approach to reduce the greenhouse gas emissions of large polluters like the steel, chemical and cement industries. In order to develop gas storage techniques in geological formations it is crucial that we can describe and monitor the associated multiphase flows. Micro computed tomography (Micro CT,

X-ray technology) has opened up new opportunities to analyse the behaviour of gases and fluids inside the porous media at high resolutions reaching sub-pore level. However, measuring in-situ pore pressures is still particularly challenging. Xenon (Xe) is a heavy, non radioactive, inert, ideal gas already used as a tracer [1,4,2]. In this study performed in a micro CT scan, energy level dependent, linear Xenon pressure- attenuation curves have been derived at different scales from static, single gas phase experiments in a Bentheimer sandstone core.

Xenon is confirmed to have a potential to function as a pressure indicator on the basis of its high atomic mass. Earlier research in a low-resolution medical CT-scan (sub porelevel) has been confirmed [5], but now by analyzing images at the pore level in a Xe-pressurized core between 0-25bar Xe, with 5μm resolution, see the Figure attached (Xenon void core Prange3.png). Material and geometry dependent artifacts as pseudo-enhancement [3] were observed. They prevent for this moment the universal use of the obtained calibration curves, though specified to the used material and set-up, the curves prove great potential. The static pressure-attenuation calibration relations are aimed to be the starting point of a method to describe pressures in static and dynamic multiphase flow in porous media.

Figure: Xenon void core Prange3.png
caption: The pressure dependence of Xenon visualized by microCT scannning of a void space in a plastic ring and a cylindrical Bentheimer sandstone core, both seen in A. The resulting cross sections of the void space and the Bentheimer core at pressure levels of 1, 15 and 25 bar are presented in B. and C. respectively. Though hardly visible in the picture, the measured Xenon signal in the pores of the core differs from the void signal at the same pressure as a consequence of pseudo-enhancement. At 15 and 25 bar the Xenon in the pores has a higher (brighter) signal than the sand grains around, opposite to the image at 1 bar.

Participation:

In-Person

References:

1 S. Akin and A. R. Kovscek. "Computed tomography in petroleum engineering research". In: Geological Society Special Publication 215 (2003), pp. 23–38. issn: 03058719. doi: 10.1144/GSL.SP.2003.215.01.03.
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Energy Transition Focused Abstracts:

810

The application of focused ion beam scanning electron microscope (FIB-SEM) to the nanometer-sized pores in shales

Author: Yunfei Zhang[1]

Co-authors: Zhaojie Song [1]; Lichao Zhang [1]; Yufan Meng [1]

[1] *Unconventional Petroleum Research Institute*

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Focused ion beam scanning electron microscope (FIB-SEM) provides a new method to study the pore structure at the nanoscale of shale, which uses gallium ion beam to serially cut the samples and simultaneously image them under electron beam, not only with high resolution but also avoids artificial pores generated during the preparation process, which can realistically reduce the 3D structural features of pores in shale and provide a useful tool for quantitative analysis of shale porosity and pore structure. FIB-SEM images were segmented with three-dimensional reconstruction using avizo software. The voxels of interest were first selected and the images were segmented using the thresholding tool in avizo software. The high-resolution secondary electron image light and darkness, which is proportional to the atomic number of the constituent elements of the sample, can clearly show the differences between shale pores, organic matter and inorganic mineral matrix in gray scale values, after the software color the three-dimensional images, it can be seen that the blue part indicates the pores, the green part indicates the organic matter, and the red and yellow parts indicate calcite and ferrihydrite, respectively. According to the above principle, the pores, organic matter, and ferrihydrite were separately extracted and their 3D spatial structures were demonstrated by manual thresholding. After that the pore network model (PNM) module of avizo software was used to analyze the pore structure. The type of data stored by a PNM module represents a grid constructed from multiple linear lines in three-dimensional space, branches or endpoints of the grid represent pores, and the line connecting the pores is called the throat. For each pore and throat, parameters such as radius, length of the throat, coordination number can be calculated. In this paper, three different types of shale samples were observed, among which red is open pores, which can be connected, blue is closed pores, that is, after the reservoir fracturing can be connected, It has been shown that the felsic shale with intergranular pores is interconnected into a large-area pore network, with several traversing crevices and wide percolation channels; dolomitic shale connectivity is intermediate between felsic shale and hybrid shale, with a few isolated pores as well as aggregate like pores; hybrid shale has a very small connection area, and the “trigonal cone-shaped” pore is connected by a “curved sheet” throat. The application of FIB-SEM to the nanopores of shale will provide new research tools for the in-depth study of shale microstructure.

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Energy Transition Focused Abstracts:

Poster / 811

Synthesis of granular activated carbon from biomass and correlation of its sorption properties with the pore space characteristics

Authors: Anastasia Stavrinou[1]; Maria Theodoropoulou[2]; Christos Aggelopoulos[3]; Christos Tsakiroglou[4]

[1] *Foundation for Research and Technology Hellas, Institute of Chemical Engineering Sciences*

[2] *Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences*

[3] *FORTH/ICE-HT*

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Granular activated carbon (GAC) produced from the thermochemical treatment of biomass wastes can be valorized as a low-cost adsorbent for the removal of various types of pollutants from water streams. Several GACs were prepared from banana peels and coffee wastes with their chemical activation by acids or alkalis and subsequent pyrolysis in a tubular furnace at temperatures ranging from 500 to 800 oC. The capacity of GACs to adsorb a mixture of a cationic (methylene blue) and an anionic (orange G) dye as well as a polyaromatic hydrocarbon (phenanthrene) was evaluated. To this direction, the sorption isotherms and kinetics were determined with batch tests and fitted with a variety of phenomenological models (e.g. Langmuir, Freundlich, 1st order, 2nd order, intraparticle diffusion). In addition, the pore structure properties of adsorbents were analyzed with Scanning-Electron-Microscopy (SEM), nitrogen sorption isotherms, and mercury intrusion porosimetry (MIP) so that the pore volume distribution over the macro-, meso-, and micro-pore sizes, along with the specific surface area distribution among the external surface of particles and internal pore surface were determined (Fig.1). This information was utilized to simulate the dynamics of pollutant sorption on the pore structure of GAC with the multi-compartment model so that the external and internal mass-transfer coefficients along with the effective pore and surface diffusion coefficients were estimated with inverse modeling. In this manner, the rate-controlling step of sorption process was correlated with GAC characteristics, pollutant type, and sorption conditions. The potential to regenerate the adsorbents by cold plasma was also investigated, and the various types of GAC were classified with respect to their sorption efficiency, and energy cost of production and regeneration.

Acknowledgments
This research has been co-financed by the European Regional Development Fund of the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH –CREATE –INNOVATE (project code: MIS 5048541; project title: "Development of a mobile ozonation unit for the remediation of polluted soils and oil-drilling cuttings").

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Energy Transition Focused Abstracts:

Poster / 812

Underground hydrogen storage in deep aquifers with CO2 as a cushion gas

Author: Sabrine BEN RHOUMA[1]

Co-authors: Daniel BROSETA [2]; Roland MASSON [3]; Farid SMAI [1]; Fernanda De Mesquita Lobo Veloso [1]; alexandre dossantos [4]; Pierre Chiquet [4]

[1] *BRGM*

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Hydrogen is regarded as a key element of the energy transition, provided it is generated from renewables and/or decarbonized energies. Since this production is estimated to be intermittent as that of renewable electricity, safe storage of large quantities of H2 needs to be considered. Currently, hydrogen storages are operated in salt caverns. However, deep saline aquifers offer medium to very large storage capacities, as well as a wide geographic distribution. Therefore, this work aims to improve the evaluation of the performance and safety of the storage of hydrogen in deep aquifers, in combination with CO2 as a cushion gas (CG).

One of the encountered challenges in this topic is to understand the degree and extent of the mixing zone between hydrogen and the CG, or the spreading of the front between these fluids. This understanding serves to minimize and control the mixing process considering that the extent of this zone impacts directly the recovery ratio and the purity of hydrogen produced. Therefore, an accurate description of the fluid mixture between the different components and their behavior within the reservoir is needed during the numerical simulation.

The relevant multi-compositional multi-phase flow requires a robust equation of state that is efficient over a wide range of temperatures and pressures and particularly around the storage conditions of the reservoir. Here, we study the different possible thermodynamic models (the research is oriented to cubic Equation-of-State (EoS) and the GERG-2008 equation) and their ability to predict the behavior of compounds of interest separately as well as the possibly resulted mixture.

Through this task and based on the experimental data collected for this system, the phase diagram of the mixture was examined with the attempt to delineate the optimum reservoir conditions, i.e., pressure, temperature and architecture that would rather curtail the mixing phenomena and promotes for the recovery of a hydrogen-rich gas (< 5% CO2). Under the proposed reservoir configurations, different scenarios are evaluated to suggest the suitable injection configuration that could possibly limit the occurrence of miscible or immiscible viscous fingering and could control the stability of the front between the fluids to curtail mixing.

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In-Person

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Energy Transition Focused Abstracts:

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813

The influence of depletion rate on the thermodynamics of retrograde gas condensates

Authors: Desmond Dorhjie[1]; Timur Aminev[1]; Alexey Cheremisin[1]

[1] *Skolkovo Institute of Science and Technology*

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Energy sources are expected to shift away from carbon-intense sources as global policies to combat climate change emerge. Natural gas resources and gas-condensate are projected to be valuable in the energy transition and remain the dominant energy source for the foreseeable future due to a lower carbon footprint compared to other fossil energy sources such as coal and oil. However, the exploitation of gas condensate reservoirs faces many challenges.

During the production of gas condensate reservoirs, a condensate bank around the wellbore region is formed when the pressure declines below the gas dew point pressure. The condensate bank resists the gas flow to the well and traps heavier hydrocarbon components, reducing the production of the wells. To improve the production index of gas condensate reservoirs, different techniques have been adopted. The existing reservoir modeling techniques utilize equilibrium cubic equations of state (EOS) for estimating the condensate and gas phases for a given pressure and temperature. However, many studies have indicated that for volatile systems such as gas condensate, the phase transition could be a non-equilibrium process depending on the rate of pressure drop.

In this study, a steady-state slim-tube experiment based on high-pressure depletion rate (HPDR) at 16 atm/hr and low-pressure depletion rate (LPDR) at 8 atm/hr was conducted. A three-component gas-condensate mixture (methane: 80.3%, butane: 13%, and decane: 6.7%) was used in the experiment at reservoir conditions or 40 ℃. The pressure was reduced from 35 MPa to 10 MPa. Furthermore, a hydrodynamic model based on equilibrium EOS was simulated to mimic the slimtube experiment.

The mass ratios of the lighter components (methane and butane) produced from the experiment agree well with the results of the equilibrium numerical simulation for both HPDR and LPDR. However, a deviation in the mass ratio of the heavier component (decane) was recorded for the HPDR experiment. This shows that an equilibrium phase transition is associated with all components of the gas-condensate mixture when a low depletion rate is applied. However, at higher depletion rates (HPDR), the non-equilibrium phase transition is recorded for the heavier components. Further analysis of the deviation between the HPDR experiment and the numerical simulation shows good agreement between them from the initial pressure through the dew point pressure until the pressure of maximum liquid saturation. Beyond the pressure of maximum liquid saturation, the deviation between the two became more significant with increasing and decreasing pressure, with the highest deviation, recorded for the lowest simulated pressure (10 MPa). This indicates that condensation (condensate formation) in a porous medium is an equilibrium process. In contrast, the process of re-evaporation is associated with a non-equilibrium phase transition.

The deviation of the mass ratio of the heavier component is expressed as a dimensionless relaxation time that can be implemented as a correction factor in equilibrium hydrodynamic simulators for the accurate prediction of condensate saturation in porous media.

Participation:

Online

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Energy Transition Focused Abstracts:

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MS06-A / 814

Nonequilibrium and cooperative behavior in quasistatic fluid-fluid displacements underpin energy dissipation and hysteresis in the passage through constrictions

Authors: Ran Holtzman[1]; Marco Dentz[2]; Marcel Moura[3]; Ramon Planet[4]; Jordi Ortin[4]

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[2] *IDAEA-CSIC*

[3] *PoreLab - University of Oslo*

[4] *Universitat de Barcelona*

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We examine the nonequilibrium nature of fluid displacement in heterogeneous media from a theoretical, numerical and experimental standpoint, using an imperfect Hele-Shaw cell featuring a localized extended constriction. We focus on the configurational energy dissipated in imbibition and drainage, and how it relates to the capillary pressure-saturation hysteresis cycle. Individual constrictions can be classified as weak (reversible) or strong (dissipative), depending on their cross-section gradient. We show however that cooperative effects can make displacements through a pair of weak defects dissipative, through spatial interactions mediated by interfacial tension; we identify the critical distance between the weak constrictions, below which irreversibility, dissipation, and hysteresis emerges.

Participation:

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References:

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Energy Transition Focused Abstracts:

Poster / 815

Direct Numerical Simulation of weak-inertia single-phase flow in porous materials using SPH

Author: David Krach[1]

Co-author: Holger Steeb [2]

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Instrinsic permeability of a porous material is a crucial material parameter in various application fields like e.g. geosciences, materials science and mechanical engineering. In these disciplines intrinsic permeability is a widley used input parameter for numerical simulations in the framework of continuum-scale models that employ Darcy's law. However, the assumption of linearity in constitutive relations for the momentum exchange is subjected to restrictions and only valid in the so-called creeping flow regime (Reynolds number Re < 1). We present an approach focusing on 3-D pore-scale-resolved computations of single-phase fluid flow through porous media from moderate to higher Re-numbers (1 < Re < 1000) aiming to show a smooth transition of effective properties from creeping flow to the weak inertia regime. While this has already been shown for 2-D artificial domains [4], we seek to generalize the phenomena by investigating spherepackings and natural porous materials with small to moderate porosities ($\varphi \leq 0.2$). For representative 3-D simulations based on XRCT-scans, with voxels in the order of 10003 massively parallel direct numerical simulation methods are required. Therefore, we choose fully-Lagrangian Smoothed Particle Hydrodynamics (SPH) as a simulation method to model pore-scale-resolved flow by means of the weakly compressible Navier-Stokes equations. The solver is implemented on top of the software framework HOOMD-Blue [1, 2] since this allows for massively parallel CPU and GPU computations. A sufficient scaling behavior as well as the numerical accuracy in the Darcy regime is demonstrated [3].

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS15 / 817

Imaging upscaling study for porosity and permeability characterization in carbonate rock using machine learning

Author: Wen Pin Yong[1]

Co-authors: Hannah Menke [2]; Julien Maes [2]; Helen Lewis [2]; Jim Buckman [2]; Sebastian Geiger ; Zainol Affendi Abu Bakar [3]; Kamaljit Singh [2]

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Porosity and permeability are vital reservoir parameters for predicting CO2 storage capacity and CO2 plume migration during CO2 storage. Apart from conventional routine core analysis (RCA) method, digital core analysis (DCA) can be applied to characterise the petrophysical and geological properties. With the advancement of computed-tomography equipment development and breakthrough in computational processing time, DCA applications can be improved using high resolution scanning combined with pore scale simulation in rock samples with single-scale porosities. However, carbonate reservoir samples are often multiscale, and therefore regardless of how sophisticated the scanning equipment, less than 1% by volume of a rock sample can be imaged at the smallest scale due to the trade-off between resolution and field of view. It is thus necessary to intelligently extract the most important features of these different scale images and combine them in a upscaled image for accurate modelling.

In this paper, we present an upscaling proof-of-concept that combines experimental scanning, subvolume extractions, machine learning regression analysis and pore-scale simulations. A CO2 storage carbonate sample was scanned using micro-computed tomography (micro-CT), SEM and synchrotron light source to understand the pore scale structure in carbonate samples at different length scales. The images were divided into smaller sub-volumes and permeability was computed and compared between the Darcy-Brinkman-Stokes (DBS) model using our in-house open-source pore scale simulator, GeoChemFoam and a commercial pore network model. A porosity-permeability relationship was first established at smaller scale. Then, the structural attributes of bigger scale sub-volumes were extracted and regressed to generate an upscaled porosity-permeability relationship. In addition, sensitivity studies were conducted to identify the optimised sub-volume size at different scales so that enough information can be captured in both the nano and micron scale porosity structures for regression analysis to quantify the properties influencing flow and create an accurate upscaled model. In this study, we found that machine learning regression is an effective technique to upscale multiscale carbonate from pore scale to micro scale. However, an appropriate choice of feature vectors especially the connectivity information is the most important feature to be included in the models. The choice of representative sub-volume size must be carefully considered during the machine learning upscaling study in order to capture sufficient structural heterogeneity to characterise different range of flow heterogeneities in the rock.

Participation:

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Energy Transition Focused Abstracts:

Poster / 818

Morphologically-stable two-phase displacements through localized constrictions are strongly dependent on flow rate

Author: Jordi Ortín[1]

Co-authors: Ido Lavi [2]; Lauren Rose [3]; Ramon Planet [2]; Jaume Casademunt [2]; Stéphane Santucci [3]

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We study imbibition and drainage through a localised constriction in a Hele-Shaw cell, as a model system designed to gain insight into multiphase displacements in porous media. In this context, the detailed quantitative response of the non-local interface dynamics to localised defects at nonzero flow rate is a key feature that remains poorly understood. Combining experiments, numerical simulations, and theory, here we show that steady conformations of a moving two-phase interface are strongly affected by the imposed flow rate, leading to asymmetric imbibition–drainage hysteresis cycles. The present results show also that medium heterogeneities can lead to long fluid filaments, and even pinch-off scenarios and fluid trapping, under linearly-stable Saffman-Taylor conditions, an insight that should be considered in practical applications of multi-phase flows through disordered media.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 821

Heat transfer through pore space in packed beds of non-spherical particles

Author: Simson Julian Rodrigues[1]

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Packed beds or granular systems and sintered or fibrous porous media are of specific interest in geosciences, the chemical industry, battery technologies and electrochemical cells. In these systems, the geometry and size of the pore space depends on the particle shape 1. Heat transport through the porous packed beds strongly depends on the tortuosity of the pore space, as it forms a resistance for gas transport. Tortuosity itself depends on porosity, specific surface area and pore morphology [2,3]. There have been several attempts to find correlations and dependency of physical parameters on tortuosity, but the results are very specific and no universal approach has been derived. In this work, the new particle parameters sphericity and aspect ratio are introduced to a correlation from [4] that yet included only a function on porosity. To achieve this, particle beds of different particle shapes and aspect ratios were created using Blender software with a rigid body simulation tool. Steady-state thermal simulations of heat conduction through the packed beds were carried out using the finite element method in software ANSYS. The heat flux results obtained were compared with the equation from [4,5] and utilized to develop the correlations with sphericity and aspect ratio.

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Energy Transition Focused Abstracts:

MS13 / **822**

Dynamical and thermodynamic aspects of evaporation of solutions from nanoporous media

Authors: joachim trosseille[None]; HUGO BELLEZZA[None]; Sujeet Dutta[1]; Olivier Vincent[2]

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Water condensation and evaporation from saline porous materials has attracted the attention of scientists for years due to a large field of applications: salt weathering of buildings, desalination of water, CO2 sequestration, soil decontamination, etc⋯[1, 2, 3]. A complete understanding of related

nanoscale processes is however lacking, in particular concerning the coupling between evaporation/condensation and crystallization/deliquescence in confinement [4]. While the comprehension of the phenomenon has progressed in the past few years [4, 5, 6], there are still some challenges remaining in characterizing and understanding these processes.

Here we carried out thermodynamic experiments coupling sorption isotherms of nanoporous media containing salt, to dynamical measurement of the evaporation of salt solution droplets from the surface of the same nanoporous media. We show that we can account for both thermodynamic and dynamical experiments by using a minimal model involving coupled phase change of the solvent (water evaporation) and the solute (salt crystallization).

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Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS11 / 823

Displacement enhancement by nanogel-in-oil suspension with macroemulsion evolution in porous media

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Nanogel particles are emerging as an attractive additive for multiphase displacement control in natural processes and engineering systems. However, different from microgel or inorganic nanoparticles, the performance and mechanism of nanogel particle suspensions have not been well explored yet. In this study, we discovered a novel nanogel-in-oil colloidal state formed naturally with ideal sphericity and long-term stability, and characterized its impact on suspension and interfacial properties. In microfluidic experiments, visualization and quantification of the displacement process revealed the enhanced displacement mode from particle retention and flow field fluctuation, to aqueous ganglion breakup and in-situ formation of macroemulsions. Non-monotonic concentration effect was explained by the pressure difference and emulsion state evolution. Comparative batch experiments were further performed to elucidate the unique property of nanogel-in-oil suspension. Our results shed light on the relationship between colloidal state of nanogel particle suspensions and multiphase displacement consequences, deepening understanding of multiphase dispersed systems.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS11 / 824

Clogging and particle accumulation during the flow of suspensions of solid particles in model 2D porous media.

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Co-authors: Youness Soumane ; Antoine Naillon

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We are interested in the transport of solid particle suspensions in porous media, which are important in many applications, in soil mechanics, in filtering operations... etc. . The accumulation of these particles is indeed often undesirable because it leads to a reduction of the permeability and sometimes to a complete clogging of the medium. Different types of clogging (geometrical, bridging, aggregation...) have been described at the pore scale, upscaling is a real issue for these phenomena.

We have designed model experiments in 2D micromodels made with standard microfluidic techniques (PDMS and glass), at an intermediate scale consisting of about 100 x 100 pores, but keeping the resolution at the pore scale. The pore geometries consist of irregular pillars, with pore diameters of 50 micrometers, i.e. a few particle diameters. Using direct fluorescence imaging, we calculate the dynamics of the local volume fraction of particles after injection of a suspension at a controlled pressure or flow rate. Importantly, we used particles with matching index and density, which not only allows good imaging but also neglects colloidal interactions.

We systematically varied particle size, concentration, and flow rate (or pressure), and observed, in agreement with single-pore studies, that the ratio of particle diameter to pore throat diameter is most important. Below 0.2, only a few pores are clogged, whereas all experiments lead to complete clogging above 0.4. In this intermediate regime where clogging is mainly initiated by geometric bridging of some pores, we observe the formation of clusters of arrested particles. The size of these clusters increases very slowly with time until reaching either a steady state or percolation. It also depends strictly on the volume fraction of the particles. Remarkably, the size of the clusters correlates well with the total fraction of the medium occupied by the arrested particles, suggesting that the percolation theory could adequately describe the clogging. In contrast, flow rate (or pressure) has only a weak effect on the observations, which we interpret as a consequence of weak particle-to-particle and particle-to-wall interactions.

Despite its weak effect in steady state, the pressure drop has a striking influence when varied over time. Periodic experiments under similar conditions lead to the conclusion that the probability of clogging is significantly reduced in the presence of flow oscillations. In regimes where clogging

does not occur in the steady state, these oscillations also reduce the particle accumulation and mean cluster size. Pressure oscillations must be of sufficiently high amplitude (typically 20% of the mean value) and of sufficiently low frequency to be used to prevent clogging of the device.

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In-Person

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Energy Transition Focused Abstracts:

MS14 / 825

Dynamic Mode Decomposition for model reduction of flow and transport in porous media

Authors: Valentina Ciriello[1]; Giulia Libero[1]; Daniel Tartakovsky[2]

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Reduced-order models (ROMs) can be used in place of a high-fidelity model (HFM) to alleviate the computational cost associated with HFM simulations. Emulators or surrogates are a class of ROMs whose aim is to reduce the complexity of a given HFM by learning the dynamics of the state variables directly from the model's output, i.e. they are trained on a dataset generated by running the HFM multiple times. As such, the number of simulations required to train a ROM is a measure of its effectiveness. Here, we use dynamic mode decomposition (DMD), a powerful data-driven method to construct ROMs of complex dynamical systems [1,2]. DMD employs singular value decomposition (SVD) and pursues the computation of the best-fit linear operator to approximate the relationship between time-shifted snapshots in time of the state variable [2]. Variants of the standard DMD algorithm exist, including the residual, generalized, and extended DMD [2,3]. In this study, we assess the accuracy of different DMD algorithms when mimicking flow and transport in porous media. We consider both interpolation and extrapolation (i.e. to get short-time future prediction) scenarios. The DMD has proven its utility in approximating systems of partial differential equations (PDEs); however, it doesn't handle the possible variability in model parameters. As such, we explore how to combine DMD with the Polynomial Chaos Expansion (PCE), a family of ROMs used to approximate the response surface of a HFM in the random parameter space; this allows to obtain a ROM in terms of a polynomial relationship explaining the model response of interest as a function of the uncertain parameters, properly represented as independent random variables [4,5].

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS15 / 826

Dynamic Mode Decomposition to reconstruct and extrapolate hydrological time series

Authors: Giulia Libero[1]; Daniel Tartakovsky[2]; Valentina Ciriello[1]

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Dealing with the impacts of climate change is one of the main challenges of our times. The definition of adaptation and mitigation strategies requires the research community to provide accurate analyses on several climate-related phenomena. Data with improved spatial coverage and time resolution are currently available through satellite technologies though interpretative efforts are needed to capture the hidden information embedded in the large amount of data collected. The dynamic mode decomposition (DMD) is a data-driven technique originated in the fluid dynamics community, to extract coherent structures from spatiotemporal complex fluid flow data 1. Similarly, if we consider a time series of observed data at a grid of spatial locations, i.e. two-dimensional field data collected at different times, the DMD method provides the leading eigendecomposition of the best-fit linear operator to approximate the relationship between time-shifted snapshots of the variable observed. The DMD method embeds automatically seasonal variations and if each location's time series is normalized in mean and variance, the approach is equivalent to a Fourier decomposition; in addition, the real part of the DMD spectrum allows to capture exponential trends in the data [2]. A suite of DMD algorithms is available to handle different applications [2, 3]. Here, we use different DMD algorithms [2, 4] and analyze their capability to reconstruct and extrapolate time series (short-time future prediction) of soil moisture as provided by satellite technologies. Soil moisture plays a major role in the water cycle and its knowledge is relevant for a large number of applications such as climate forecasting, water resources and ecosystem management, drought and flood. The dataset analyzed in this study is produced on behalf of the Copernicus Climate Change Service (C3S); soil moisture data are provided on a global regular latitude-longitude grid at a resolution of 0.25 degress, with a temporal coverage from 1978 to present, on a daily and monthly scale [5].

Participation:

In-Person

References:

1 P. J. Schmid, Dynamic mode decomposition of numerical and experimental data, Journal of Fluid Mechanics 656 (2010) 5–28. doi:10.1017/s0022112010001217.
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Energy Transition Focused Abstracts:

MS08 / **827**

Pulsed Flow Injection Strategies for Enhancing Subsurface Mixing

Authors: James Minto[1]; Gloria Castro[2]; Jen Roberts[1]

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[2] *Postdoctoral researcher, Civil and Environmental Engineering, University of Strathclyde*

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Pulsed flow has been proposed as a means of enhancing mixing in porous media. Compared to diffusion alone, a zero time-averaged advective flow has been found to accelerate mixing by hundreds to thousands of times1. There are many potential applications where this would be beneficial, for instance remediation of subsurface contamination, open-loop geothermal, ground improvement by grouting, and even when making the perfect shot of espresso. The pumps used for these applications typically produce flow that pulses to some degree, the nature of which depends on the pump mode of operation, the required flow rate, and properties of the porous media such as permeability, network connectivity, and the systems compressibility.

In this research, we explore the implications of pulsed flow on transport and mixing in porous media seeking to understand how injection strategies can incorporate deliberate flow pulsing so as to enhance mixing.

Methods:
The pressure pulse characteristics of several common pumps were measured: lab-scale syringe, piston and peristaltic pumps, field-scale screw and diaphragm pumps, and a home espresso machine. OpenFOAM was used to model flow and transport through i) a set of individual stylised pores, ii) a 2D pore network, and iii) a 3D X-ray scan of a sand packed column. Representative pressure pulse profiles were used as the inlet boundary condition to these pore-scale numerical models.
To validate the numerical model, a complementary microfluidic experiment was carried out in which transport of a fluorescent tracer through a stylised 2D pore was observed under pulsed and non-pulsing flow.

Results:
Model results indicate that flow/pressure pulsing has a relatively minor effect on pore-scale mixing

under truly laminar conditions, however mixing becomes more pronounced as flow becomes transitional (pore Reynolds numbers >10) due to enhanced mixing in dead-end pores. Likewise, mixing is enhanced substantially in a multiphase system when the stationary phase is compressible, for instance water injected into an initially dry or partially saturated rock/soil/coffee.

There are clearly scenarios in which a pulsed injection strategy could be adopted so as to reduce the total time or the total injected volume required to mobilise a pollutant and, equally, there are scenarios in which pulsed flow will have little impact.

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MS09 / 828

Pore-network modeling of gas hydrate dissociation: impact on pressure response and gas transport

Authors: Chico Sambo[1]; Karsten Thompson[None]; Olufemi Olorode[1]

[1] *Louisiana State University*

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Naturally occurring methane hydrates are a world-wide occurrence from the arctic permafrost to the continental shelves in tropical areas. Methane hydrates have the potential to be produced as an energy resource. Additionally, they can undergo phase transition (formation or dissociation) as a result of changing environmental conditions, and predicting the behavior is important for design of subsea infrastructure, predicting submarine slope instabilities, and understanding climate impacts from gas evolution. To this end, we are studying hydrate behavior using a multiscale model that integrates molecular-scale, pore-scale, and Darcy-scale behavior. This multiscale approach connects the fundamentals (e.g., thermodynamics and kinetics of hydrate formation, and pore-scale structure and hydrodynamics) to larger scales, in a way that is not possible using current empirical approaches.

In this talk, we focus primarily on the pore scale, and specifically modeling the dynamic phase change and fluid transport that occurs as methane hydrate dissociates due to changes in pressure or temperature. The pore-structure and spatial distribution of hydrate is obtained from microtomography images. The pore-scale distribution of hydrate interfacial area and its evolution as a function of hydrate saturation is also predicted from analysis of the digital images. The dissociation kinetics are obtained from molecular dynamics (MD) modeling and upscaled to the pore scale by computing an interfacial velocity for dissociation. The resulting pressure response and fluid transport is modeled

using a novel pore-scale model derived from a time-dependent mass balance, and which accounts for both fluid compressibility and phase change.

Initial results from this work include MD simulation studies, which quantify the thermodynamic stability and dissociation kinetics. The pore-scale model for compressible flow with phase change is validated using known Darcy-scale results under simple conditions. It is then extended to incorporate dynamic dissociation behavior upscaled from the MD simulation studies. The resulting model is used to quantify the pressure response and gas transport that occurs as a result of pressure drop or temperature rise. Finally, we propose how these results can be upscaled to provide quantitative parameters for meter-scale or km-scale modeling.

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Energy Transition Focused Abstracts:

Poster / 829

Laboratory scale demonstration of asbestos mobility in sandy aquifer systems

Author: Leonardo Magherini[1]

Co-authors: Chiara Avataneo ; Silvana Capella ; Manuela Lasagna ; Carlo Bianco [2]; Elena Belluso ; Domenico De Luca ; Rajandrea Sethi [1]

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Asbestos is a well-known and regulated air pollutant and it is indeed classified as a carcinogenic compound of the first group. However, several studies recently reported asbestos presence also in fresh water sources, such as lakes, rivers, groundwater and drinking water. As far as human exposure, two main pathways can be identified for waterborne asbestos: (i) inhalation due to water evaporation and subsequent fibre dispersion into air; (ii) ingestion mainly via drinking water. For the first case, the concentration limits (number per litre of longer than 5 μm fibres) established for air must be respected, i.e. 100 f/L at workplaces (U.S. Occupational Safety and Health Administration) and 1 f/L in outdoor environments (World Health Organization). As for oral exposure, the effects of asbestos ingestion on human health are still not well known; however, the U.S-Environmental Protection Agency established a precautionary concentration limit for longer than 10 μm fibres in drinking water of 7·10⁶ f/L.
Focussing on groundwater contamination, asbestos fibres can typically be found in areas where water flows through aquifers containing Naturally Occurring Asbestos or in the proximity of mines and mine tailing deposits. The abovementioned contamination scenarios can represent a severe environmental and sanitary issue due to the potential capability of asbestos to migrate through aquifer systems. However, until now asbestos has been considered substantially immobile in groundwater

since its shape and surface charge are expected to result in irreversible filtration of the fibres upon release into the aquifer. Therefore, no studies have investigated in depth the mechanisms governing the asbestos subsurface mobility so far.
This laboratory scale work studied the transport of crocidolite, a negative charged amphibole asbestos, through quartz sandy aquifers. Two sets of column tests were performed varying the concentration of the injected asbestos suspension, the sand grain size distribution and the water pH. The asbestos concentration in water was measured at the column inlet and outlet using a UV-vis spectrophotometer and the fibre number, size and shape were characterized through SEM-EDS analysis. The results demonstrated that crocidolite asbestos is not actually immobile and can potentially flow through sandy porous media. As expected, fibre retention was higher in the finer sand, even if the grain size influence was found to be more pronounced when increasing asbestos concentration in the injected suspension. Interestingly, the study showed that asbestos deposition is not completely irreversible, since a fraction of the filtered fibres was remobilized after the column was flushed with high pH water. As for morphological characterization, small fibres proved more mobile than the long ones: several fibres with length > 5 μm (carcinogenic when respired) were collected at the column outlet, whereas most of the fibres longer than 10 μm were filtered out by the porous medium. These results suggest that the air dispersion of waterborne fibres is expected to be the most likely and impacting scenario. Future studies should therefore aim at confirming the effective crocidolite mobility also in real environments.

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Energy Transition Focused Abstracts:

830

Wettability of Supercritical Carbon Dioxide, Brine, and Shale as a Function of Pressure

Authors: Deepak Tapriyal[1]; Foad Haeri[1]; Dustin Crandall[2]; Angela Goodman[1]

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Injection of large amounts of carbon dioxide (CO2) into subsurface reservoirs for geologic carbon storage will increase the pressure in these reservoirs and surrounding zones. Due to buoyancy, the CO2 will gradually migrate upwards towards low permeability sealing formations (e.g., shales) above more porous injection zones. These seals must restrict further vertical movement of the CO2 to groundwater and the surface for geologic carbon storage to be a viable method of substantially reducing anthropogenic greenhouse gas emissions. Using a unique precision experimental device, we have examined the change of CO2/brine/shale contact angles under representative carbon storage scenarios. Shale samples were submerged in brine, system temperature was maintained at 40℃ or 100℃, and pressure of the system was increased from 8.3 MPa to 62 MPa. After equilibration, small bubbles of supercritical CO2 (diameters ranging from 200 to 2200 microns) were placed below the

shale samples submerged in brine and the contact angle of the CO2 was measured. No significant alteration of the contact angles was observed due to changes in temperature or pressure, though smaller bubbles did tend to have slightly higher contact angles, as has been previously reported (Haeri et al 2021). There was no observed change of the wettability from water wetting to CO2 wetting, which bodes well for sustainable CO2 storage in geologic carbon storage reservoirs as the pressure increases from large volume injections.

Participation:

Online

References:

Haeri, F., Tapriyal, D., Matranga, C., Crandall, D., Goodman, A. (2021) Variation of CO2-Brine Contact Angles on Natural Rocks of Different Compositions J of Energy and Power Technology, 3(4):14; doi:10.21926/jept.2104046

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Energy Transition Focused Abstracts:

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MS17 / **831**

Monte Carlo method to solve the heat equation in a complex media

Authors: Alicia Laroche[1]; Jose Luis Limon Farfan[2]; Simon Eibner[3]; Stéphane Blanco[4]; Christophe Coustet[5]; Mouna El Hafi[1]; Richard Fournier[4]; Benjamin Piaud[5]; Frédéric Topin[6]

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Porous or fibrous complex medias are widely used for energy applications such as heat storage, thermal insulation, solar absorbers, heat exchangers… There is a need to develop methods that are relevant to solve the heat equation in those complex medias.

Monte Carlo method can be used to solve parabolic partial differential equations such as heat equation in complex geometries [1,2,3] or porous media. It relies on reformulating the thermal model first as an integral and then as an expected value introducing a probability density function. An important point is that this method does not require a volumic mesh which makes it relevant for complex geometries.

Randomly generated paths carry information (known temperature or flux on a boundary, volumetric heat source...) in their weights.The observable - local temperature, mean temperature on a given surface - is then evaluated by computing the arithmetic mean of the weights, based on the Law of Large Numbers. It is noticeable that Monte Carlo method does not evaluate a temperature field but only the observable. Therefore, it reduces the amount of data to handle for post-treatment. The Monte Carlo algorithm can easily be parallelized since each path is independently computed on a single processor. Based on the Central Limit Theorem, the result is always given with its variance and then with the associated uncertainty.

In this work, we solve the thermal model in a diphasic complex porous media.
Geometry has been obtained through tomography technique and is composed of 8×10^6 triangles. This sample has been chosen for its complexity: large range of spatial scales, hollow fibres... Computations have been performed with the free and open-source software Stardis (https://www.meso-star.com/projects/stardis/stardis.html) which is suitable to take conduction, convection and radiation transfers into account. Based on recent work of Tregan [4], Stardis has been extended to non-linear cases to take the radiative term - difference of temperatures to the power four - into account without linearization which is crucial when the difference of temperatures is high.In the present work, the thermal model has been successfully solved to determine the apparent conductivity tensor with and without radiative transfers.

Further work is required to investigate how to solve other advection-diffusion equations with this Monte-Carlo method.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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MS01 / 833

Influence of Capillarity on Salt Precipitation during Primary CO2-Brine Displacement

Authors: Boris Jammernegg[None]; Denis Martynov[None]; Theresa Schollenberger[1]; Johannes Hommel[1]; Gerald Stiedl[None]; Bernd Flemisch[1]; Holger Ott[2]

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Geological storage of CO2 is currently considered as the most promising large-scale option to avoid emissions by industrial activities. As suitable subsurface containers, oil and gas reservoirs and the more abundant saline aquifers are considered. The injection of dry or under-saturated supercritical CO2 into water-bearing formations leads to the formation of a dry-out zone due to evaporation/dissolution of the resident brine into the injected fluid and, thus, potential precipitation of formerly dissolved brine constituents. If minerals precipitate within the pore space of a rock formation, porosity and permeability are negatively affected, which potentially impairs injectivity. Even though the impairment of injectivity poses both operational and financial challenges, minor attention has been dedicated to this research area so far. What is the size of the affected zone itself? What is the impact of capillarity on the fluid transport therein?

In this presentation, the responsible evaporation of brine and fluid transport mechanisms are outlined and discussed, as well as the potential reduction of the formation permeability and with it the injectivity. A remaining important question is the zone of counter-current flow in the direction of the wellbore, which determines the amount of salt that potentially precipitates in the near-wellbore area and the accompanied porosity reduction. Current reservoir simulation tools are not accounting for this effect because they typically do not capture evaporation kinetics. Earlier studies indicate that in certain cases the respective permeability can be reduced by several orders of magnitude (Ott et al., 2021), which comes close to a loss of the injection well.

We approach this question with numerical simulations to determine the size of the zone affected by the undersaturated CO2 that allows for salt to be transported toward the injector and the major parameters governing this zone and their dependencies as well as the fluid transport therein. We are currently developing and testing a reservoir simulation module based on DuMuX capable of describing reaction kinetics. In parallel, we built up a meter-scale core flood experimental setup that allows us to extract fluid saturation profiles and solid saturation (precipitation) via CT imaging of core samples. Besides that, by monitoring the differential pressure, we can determine changes in permeability and with it changes in injectivity.

This study aims to establish an experimental/numerical workflow to forward simulate, respectively design, and to history match experiments with a reservoir simulator to upscale the results to the field scale. The work is currently in progress –the applied workflow will be outlined in detail.

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MS06-A / 836

Tortuosity-governed droplet transport in a microfluidic porous network

Authors: Elliot SPEIRS[None]; nicolas PANNACCI[1]; Maxime Moreaud[2]; Marie-Caroline Jullien[3]

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Multiphase flow in porous media is widely studied and impacts countless applications in many natural and industrial processes, such as geologic CO2 sequestration, water infiltration into soil, and particle filtration. However, many questions remain, particularly with regard to the effect of the confinement and the geometry of the porous medium on the transport of dispersions.

We address these issues experimentally using controlled porous media: micromodels. We designed polydimethylsiloxane (PDMS) micromodels consisting of regular networks of vertical cylindrical posts, at the centres of which we injected water droplets in a continuous oil phase. A priori, no preferential paths are expected, except in a stochastic manner. However, we show that the radial alignment of the posts, i.e. the geometric tortuosity of the network, varies angularly in a periodic manner and plays a key role in droplet transport by generating reproducible preferential paths. By systematically varying the geometrical configuration of the posts, injection capillary number, droplet size, and droplet concentration, we characterise the droplet transport and the conditions for droplet breakup. At low capillary numbers, radial droplet transport is homogeneous. By increasing the capillary number, droplets initially follow the least tortuous paths before transitioning to a stable flow regime whereby droplets flow primarily in the most tortuous paths. Through large-scale droplet tracking, we demonstrate the influence of the geometric tortuosity of the media on the resulting droplet flow patterns and the counter-intuitive responses that can arise. Through this analysis, we emphasise the role of local geometrical configuration and propose a new metric for droplet transport which is the tortuosity of the porous media.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS05 / 837

Using Branching Fungus to Remediate NAPLs Trapped in Hard-to-reach Areas in Fractured Porous Media

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Non-aqueous phase liquid (NAPL) trapped in stagnant or low permeability regions, such as a dead-end fracture or rock matrices, are hard to remediate because they are mostly inaccessible by groundwater flow. In this study, we utilize branching fungus to remediate NAPLs immobilized in low permeability regions. Hyphae of fungi are known to generate tremendous turgor pressure on their tips 1 and produce surfactants [2] that allow them to navigate through small pores and air pockets in porous media and even penetrate rock matrix [3]. However, to the best of our knowledge, there has been no direct visualization of fungal hyphal penetration into oil-water interfaces, and its implication on the remediation of NAPL has been unclear.

This study reports the active removal of NAPL by fungi using microfluidic experiments. We isolated naphthalene-degrading colonies from a local coal-tar-contaminated site, and through the microbiome analysis, we identified and selected the fungal colony which constituted the major fungal populations in biofilms sampled from the site. The fungi were suspended in a minimal salt medium, and the solution was injected into a PDMS microfluidic chip with a flow channel surrounded by NAPL-saturated low porosity regions (Figure A). Vegetable oil with 10 g/L of naphthalene was used as the model NAPL. The fungal growth and the change of oil-water interfaces were recorded through a scientific CMOS camera at the pore scale. Our results showed the active removal of NAPL by fungi over 65 hours. We observed that clogging of the preferential flow path by fungi induced flow instability which led to a fingering-like displacement of trapped NAPL (Figure B). Moreover, fungal hyphae effectively penetrated water-oil interfaces and significantly enhanced the oil removal from low porosity regions (Figure C). In this contribution, we will further discuss the mechanisms behind the effective removal of NAPL by fungi.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS06-B / 839

Systematic study of wettability alteration of glass surfaces by dichlorooctamethyltetrasiloxane silanization; a guide for contact angle mod-

ification

Author: Tomislav Vukovic[None]

Co-authors: Jostein Røstad [1]; Umer Farooq [2]; Ole TORSAETER [3]; Antje van der Net [4]

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Wettability plays an important role in many natural and industrial processes, like mineral processing, hydrocarbon production and ground water remediation. For multiphase fluid flow in porous media, extensive research has been performed on the influence of the wettability on the phase distribution and morphology in both, static and dynamic conditions (1,2,3,4,5). Wettability is also crucial for the topics of increasing interest - hydrogen and carbon dioxide storage, for example for the description of injection dynamics and assessment of caprock stability (6).
In order to investigate wettability effects on multiphase flow in a controlled and standardized manner, researchers utilize model systems like bead-packs or micromodels. Glass is one of the materials used for the creation of such models, being transparent, chemically inert and easily formable. Additionally, the wettability of the glass surfaces can be altered from its original hydrophilic to more hydrophobic state by reaction of silane/siloxane groups with the hydroxyl groups of glass known as silanization (10).
The degree of wettability alteration by silanization reaction depends on numerous variables (7,8,9) such as the reaction time, temperature, concentration, the nature of the solvent and the prior glass cleaning procedure. Although silanization is widely used for glass wettability modification, comparable detailed systematic approaches over a large range of geometries, treatment conditions and measurement systems are scarce in the literature (7,8,9).
In this work, dichlorooctamethyltetrasiloxane (Surfasil) treatment was investigated with the purpose of systematically obtaining and providing a guide for achieving a wide range of contact angles. Secondly it was investigated whether different geometries display comparable contact angles under similar treating conditions using independent methods of contact angle determination.
Wettability was quantified through contact angle measurements on glass plates, beads and 2D micromodels. Initially, the influence of the solvent, treatment time and Surfasil to solvent ratio on plates was investigated using the sessile drop method. After establishing a clear relationship between the parameters and contact angles, the same treatment parameters were applied to single bead, microchip and multiple glass beads, the latter to form a bead pack. Contact angles from single beads and micromodels were obtained using image analysis of projections, while contact angles within the bead-pack were extracted from segmented 3D micro-CT images using algorithms (11).
By varying treatment times and the Surfasil to heptane ratio, it was possible to achieve a wide range of comparable and repeatable contact angles; from the initial 20 to 100 degrees as ultimate non-wetting state measured for air-water systems; for plates and individual beads, see figure attached. The flooding treatment in the micromodel was so far limited to the ultimate non-wetting state, showing comparable results to the plate and individual beads within limitations of the measurement.
Contact angle derivations from the bead pack using the 3D micro-CT images showed higher contact angles in comparison to the single bead, but it confirms a larger spread of the contact angle as observed in the literature (12).

Figure caption: The dependency of the contact angle on the volume ratio. The contact angle increases until it reaches a plateau value.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 840

Towards a clinically relevant porous media model for vertebroplasty

Authors: Zubin Trivedi[None]; Jan-Sören Völter[1]; Arndt Wagner[1]; Tim Ricken[1]; Oliver Röhrle[1]

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More than 1.4 million clinical vertebral fractures occur annually, making them a common occurrence worldwide. The cause of vertebral fractures could be injuries resulting from accidents or osteoporosis in old age. Vertebroplasty is a commonly used procedure to treat and prevent vertebral fractures. The procedure involves injecting bone cement inside the vertebra and letting it harden by curing.

One of the risks associated with the procedure is leakage of bone cement into blood vessels or the spinal canal, leading to complications like pulmonary embolism, paralysis, etc. The outcome of the procedure is often hard to predict because of uncertain factors like the unknown trabecular structure, non-Newtonian nature of the bone cement and the bone marrow, curing of the bone cement, etc. A computational model that can simulate the procedure could be a useful tool for surgeons.

We have developed a multiphase continuum-mechanical macro-scale model based on the Theory of Porous Media for simulating vertebroplasty. The related governing equations were discretized using a combined Finite Element - Finite Volume approach by the so-called Box discretization. Different rheological models for upscaling the non-Newtonian rheologies were used to compare and determine the most suitable one for this application. The model was validated using a benchmark experiment that was set up physically and in simulation. The influence of bone marrow and parameters like permeability, porosity, etc. was investigated to study the effect of varying conditions on vertebroplasty. We found that the presented model could realistically simulate the injection of bone cement in porous materials when used with the correct rheological upscaling models.

Going forward, we want to use this model to identify and investigate the critical parameters that affect the outcome of the vertebroplasty procedure. Furthermore, the model could be extended to include the temperature effects and fractures, as well as to account for the uncertainties arising from the patient-specific nature of the various parameters. Using this model to develop a clinically relevant tool for practitioners could help them make better decisions regarding the operating parameters and conditions for each patient.

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Energy Transition Focused Abstracts:

MS15 / 841

Application of Machine Learning to Generate Multiphase Pore-Scale Images

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Machine learning has been applied successfully, using three-dimensional images as training datasets, to generate realizations of the pore space, as well as to produce super-resolution images. We extend this work, using GANs to generate images both of the pore space but also two fluid phases within the pore space, using experimental high-resolution three-dimensional X-ray images of the pore space and fluids at different fractional flows as training datasets. We demonstrate that using GANs we can generate images for a range of saturation and compare the quality of the realizations against experimental data in terms of Minkowski functionals: saturation, interfacial area, mean curvature and

connectivity (Euler characteristic) as well as contact angle. We discuss the use of this methodology to complement pore-scale displacement and imaging experiments, to generate images of arbitrary size and for a wide saturation range. These images provide a basis for further analysis and pore-scale modelling, including prediction of averaged multiphase flow properties, such as capillary pressure and relative permeability.

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Energy Transition Focused Abstracts:

MS09 / 842

Pore-scale modelling and analysis of multiphase flow in gas diffusion layers

Authors: Branko Bijeljic[1]; Jiafei Zhao[2]; Martin Blunt[1]; Min Li[1]; Sajjad Foroughi[1]

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Wettability design is of crucial importance for optimization of multiphase flow behaviour in gas diffusion layers (GDLs) in fuels cells. The accumulation of electrochemically-generated water in the GDL will impact fuel cell performance. Hence, it is necessary to understand multiphase displacement to design optimal pore structures and wettability to allow the rapid flow of gases and water in GDLs over a wide saturation range. In this work, high-resolution three-dimensional X-ray imaging combined with a pore network model was used to investigate the breakthrough capillary pressure and water saturation in gas diffusion layers manufactured with a different degree of polytetrafluoroethylene coating: 5, 20, 40, and 60%, making them more hydrophobic. We first demonstrate that the pore network extraction method provides representative networks for the fibrous porous media examined. Then, using a pore-network flow model we simulate water flooding in initially gas-filled fibrous media, and analyse the effect of wettability on breakthrough capillary pressure and water saturation. Overall, this work demonstrates that the wettability and flow direction have a significant impact on breakthrough capillary pressure and water saturation during multiphase flow in GDLs and that with an appropriate pore-scale characterization of wettability, a pore network model can match experimental results.

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In-Person

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MS07 / **843**

Modeling plant water deficit by Richards'equation with a non-local root water uptake term

Authors: Marco Berardi[1]; Giovanni Girardi[2]

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In this talk we present a novel way to mathematically frame the concept of *ecological memory* of plant water stress in the context of root water uptake in the unsaturated flow equation.
As reported in 1, ecological memory can be defined as "the degree to which an ecological process is shaped by its past modifications of a landscape". Inspired by recent eco-hydrological papers (see in particular [2], [3]), we model the water content dynamics in a soil plant system by Richards'equation with a non-local root water absorption term. In order to account for this memory term, an integral equation is defined, and sufficient conditions are provided which ensure existence and uniqueness of its solution: in particular, the memory term carries a weight function and takes into account 1) the *length* of the memory; 2) the *temporal pattern* of the memory; 3) the *strength* of the memory.
Finally, tailored numerical methods are implemented, and numerical simulations are also provided: in particular, we show the behaviors of memory terms with exponential weight and with fractional weight.

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Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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Predicting the effect of capillary heterogeneity on methane plume migration in shallow unconfined aquifers: Physics-based and surrogate modeling

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We investigate mechanisms that enhance lateral methane (CH4) plume migration in shallow aquifers that exhibit complex and multiscale heterogeneity. We show how heterogeneity in capillary pressure characteristics related to millimeter- and centimeter-scale strata results in enhanced lateral spreading of gaseous CH4, caused by retarding, deviating, and/or blocking upward buoyancy-driven CH4 migration. We also show, both qualitatively and quantitatively, that meter-scale sedimentary stratification contributes more to CH4 plume migration than the millimeter- and centimeter-scale strata comprising them. Our work shows the extent of gaseous CH4 transport, and its associated impacts on groundwater quality and global warming, cannot be accurately assessed unless the sedimentary architecture and resulting heterogeneity in capillary pressure are represented. Further, we design surrogate models, based on conditional deep convolutional generative adversarial network (cDC-GAN), to map the cross-domain between input and output pairs in a multiphase system. The cDC-GANs determine, both qualitatively and quantitatively, CH4 distribution in multiscale subsurface systems. Compared to numerical simulations, the cDC-GANs can predict spatiotemporal dynamics of CH4 plume with high accuracy. Further, for a given time, the developed cDC-GANs can instantly predict the amount of CH4 in different forms (i.e., mobile, residually trapped, dissolved, and leaked to the atmosphere). The cDC-GAN approach can be considered as a valid alternative to numerical simulations for predicting multiphase flow behavior in other geoscience-, energy-, and environmental applications such as contaminant transport, hydrocarbon production, and geological carbon dioxide and hydrogen storage.

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Energy Transition Focused Abstracts:

MS02 / 846

Characterization of evaporation induced aquifer-scale mixing and mineral precipitation

Authors: Marco Pieretti[None]; Luis Cueto-Felgueroso[1]; Elena Abarca[2]

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This study aims to investigate the interplay between mixing in porous media and mineral precipitation from groundwater. These processes are fundamental in salt lakes/lagoons, soil salinization, land desertification, alteration of soil's mechanical properties and reliability of wastewater disposal. These contexts are mainly found in arid and semi-arid regions, where the evaporation plays a key role in the coupling of those processes, as it drives upward the groundwater flow and reconcentrates the solutes at the exposed aquifer surface. The resulting increase in shallow water density consists in a gravitationally unstable condition that relaxes through the formation of saline fingers and the development of a free convective regime in the entire aquifer. In this way, solutes sink while they are precipitating as mineral phases in the intergranular pores, in case of saturated waters. Then, effects on the evaporation rate and aquifer geochemistry derive from the changes in porosity and relative amounts of chemical species. Here we present a variable-density flow model coupled to reactive transport to replicate a typical evaporite environment and the aquifer beneath, in fully saturated conditions. The numerical model simulates well the aquifer recharge according to realistic values of evaporation and permeability, meanwhile, the reconcentration of solutes and the resulting fingers of saline water that grow, merge, diffuse, and sink. Evidence of the above-mentioned diluting mechanism is visible in the periodic oscillation of maximum density in the system (i.e. linear function of the concentration) with time, which drastically decreases after a local maximum value corresponding to finger formation event. This sensitivity is observed in the mixing indicators too, while the system, started at a homogenous condition, goes through an increasing segregation to progressively recover to better mixed stages, when the salinization of the deeper aquifer is observed, and the inflow of fresh water is limited to a superficial wedge. Indeed, changes in the fingering dynamics lead to substantially different evolution of the aquifer flow and geochemistry, that is, the combination of evaporation rate and permeability, which define the boundary layer Rayleigh number (Wooding, 1997), enhancing or not the convection. We observe that for higher values of this number, the maximum density reached in the system decreases, consistently with a more dynamic evolution, faster and stronger aquifer salinization, and a thinner freshwater wedge. The model simulates adequately the precipitation of minerals within the most superficial soil layer and a complementary decrement of porosity, showing a heterogeneous spatial distribution depending on the fingering dynamic occurring beneath as well as a different amount depending on the strength of the convective regime. Thus, the numerical simulations can be implemented as a predictive reactive transport tool applied to geo-engineering and agricultural studies.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-A / 848

A simplified pore-scale model for drainage including film flow effects

Authors: Paula Reis[1]; Marcel Moura[1]; Knut Jørgen Måløy[1]; Eirik Grude Flekkøy [1]; Per Arne Rikvold[1]

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During drainage in porous media, film flow through networks of corners and capillary bridges can establish connections between seemingly isolated defending fluid clusters. Coupled with the drainage through the bulk of pores and throats, the flow through these networks constitutes a secondary drainage mechanism that can significantly affect final fluid configuration and residual saturations. We propose a simple numerical model that incorporates such mechanism by modifying the cluster identification algorithm in an invasion percolation model for drainage. In the model, which represents quasi-2D porous media, wetting-phase-filled sites are considered available to invasion when connected to the liquid outlet directly through successions of pores and throats, or through chains of interconnected capillary bridges. Within the available sites, the order of invasion follows a hierarchy of local capillary pressure thresholds that can be perturbed to accommodate gravitational and viscous effects. With the proposed model, recently obtained experimental data of drainage of Hele-Shaw cells filled with spheres were reproduced, showing good qualitative agreement. In particular, we investigated the existence of an active zone where film-flow-related events are more likely to occur, the capillary bridges size and spatial distributions, and the impact of film-flow drainage on the residual saturation.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS03 / 849

Particle deposition and clogging over rough natural fractures with surface attachments

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Particle transport in rough natural fractures has seen diversified potentials and applications in environmental engineering and resource development engineering. Despite intensive and outstanding research on their transport phenomena, the impact of surface attachment and confined space of rough natural fractures on particle transport remains poorly understood.
In this work, we simulated the transport behavior of micro-particles using a coupled computational fluid dynamics and discrete element method (CFD–DEM) approach, accounting for irreversible surface attachment and particle-particle interactions in rough fractures with spatially varying apertures. Rough fracture geometries are generated with the geostatistical simulator SgeMS by two dimensionless roughness parameters. The influence of roughness parameters and surface attachment on the flow field and micro-particles migration are investigated. Numerical results indicate that surface attachment will intensify the particle sediment and clogging over a rough fracture especially at the fracture inlet zone. As the fracture aperture gradually decreases, and the contact area increases, resulting in a more complicated flow field and transport behavior. In addition, the particle deposition rates were increased by the mean roughness and an uneven particle distribution can be observed. Rough fracture walls will not only lead to more energy loss due to frequent particle-particle and particle-fracture contact, but also resulting in an increase in the average particle velocity. The overall findings will shed light on understanding clogging and deposition characteristics of particles in subsurface rough natural fractures.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS09 / 850

Modelling the transport and retention of nanoparticles in a single partially-saturated pore in soil

Author: Jayaraj J[1]

Co-authors: Seetha N [2]; Majid Hassanizadeh S [3]

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Due to the wide application of nanotechnology in several fields including various consumer products, industrial processes, and biomedical fields, release of nanoparticles into the subsurface is inevitable. Once they enter the soil, they get transported through the vadose zone, where a fraction of the infiltrated particles is retained at grain surfaces (also called solid-water interface, SWI), air-water interface (AWI), and air-water-solid contact region (AWS). These retained particles may get remobilized due to change in water flow and chemistry making the vadose zone a secondary pollution source. Hence to evaluate groundwater pollution, it is necessary to understand the transport mechanisms of these particles in the unsaturated part of subsurface. In this study, a 3D mathematical model is developed to simulate the transport and retention of nanoparticles within a single partially-saturated pore with an angular cross-section. The model accounts for particle deposition at SWI, AWI, and AWS. A novel formulation for particle diffusive transport from AWI to AWS, where particles are assumed to be retained irreversibly by capillary forces is developed. The transport in the pore is modelled using the advection-diffusion equation and the mass exchange with the SWI, AWI and contact region are modelled as first-ordered reactions that depend on the interaction energy of particles with the interfaces. Quantitative relationships for attachment and detachment rate coefficients of nanoparticles towards various interfaces with respect to twelve different pore-scale parameters were developed. It was found that the geometry and flow parameters play a significant role in the retention of particles at various interfaces, and parameters describing the system chemistry have a negligible effect on particle retention. The formulas for attachment and detachment rate coefficients of nanoparticles towards various interfaces developed in this study can be further incorporated into a pore-network model to upscale particle transport to the continuum scale.

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References:

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Energy Transition Focused Abstracts:

MS22 / 851

Removing size effect on 3D-printed material's strength by controlling its microstructure

Author: Xinrui Zhang[1]

Co-author: Martin Lesueur

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Additive manufacturing, commonly called 3D printing, is increasingly applied in numerous disciplines. The most common type, Fused Deposition Modelling, manufactures 3D-printed parts by extruding a filament of molten material layer upon layer. Upon solidification of the molten filament which cross-section has rounded corners, air gaps are created between each layer (Biswas, Guessasma, and Li 2020). Given the presence of those air gaps, this 3D-printed material can be defined as a porous material, for which mechanical properties are then dictated by the classical laws of poromechanics. Considering the internal length scale introduced in the system via porosity, we postulate that these manufacturing imperfections influence the 3D-printed material mechanical size effect, which has been shown to exist in various studies (Bell and Siegmund 2018; Wu, Chen, and Cheeseman 2021). Here we show that this size effect can effectively vanish if air gaps and sample size are simultaneously scaled. By fine-tuning certain printing parameters such as printing speed (Lanzotti et al. 2015) and printing temperature (Afonso et al. 2021), we find it feasible to maintain the shape and distribution of air gaps while varying sample size. Given the possibility of scaling the 3D-printed material's microstructure along with the sample size, we are left to check whether this is enough to effectively remove the size effect phenomenon previously observed. From our results on cubic samples of 3D-printed polylactic acid (PLA) (Figure 1), we obtain similar stiffness (3.1% differences) and uniaxial compression strength (3.2% differences) when the microstructure is scaled with the sample size, whereas 19.8% differences in stiffness and 12.6% differences in strength are obtained when the microstructure is fixed, see Figure 2. With this study, 3D-printed material mechanical size effect can be linked to the printing parameters straight-forwardly, which is a starting point towards predicting more directly the mechanical behaviour.

Participation:

In-Person

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Energy Transition Focused Abstracts:

MS12 / 852

Simulation of cyclic storage of hydrogen in salt caverns based on laboratory-benchmarked modeling of creep

Authors: Herminio Tasinafo Honorio[1]; Maartje Houben[2]; Arjan van der Linden[2]; Kevin Bisdom[2]; Karin de Borst[2]; Lambertus J Sluys[3]; Hadi Hajibeygi[1]

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Salt caverns provide promising storage capacities for safe cyclic storage of hydrogen. With a few caverns worldwide in operation for (monotone) hydrogen storage as feedstock to chemical factories, scaling up their utilization for energy transition requires quantification of the rock salt mechanical behavior under cyclic loading. Not only the mechanics of the rock salt specimen, but also the deformation and stability of the entire cavern structure, considering the heterogeneities and uncertainties, under cyclic loading needs to be quantified [7]. Rock salts are known to have complex inelastic and time-dependent deformation mechanisms under different stress regimes, temperatures, and loading frequencies. For hydrogen operations, in which the period of injection/production scales in the order of days, transient creep (i.e. primary creep stage) is expected to play a major role, while the impact of steady-state and accelerated creep stages take place in much longer time scales.

The existing models for salt rock mechanics assume the transient creep is either fully recoverable [3,5,9] or fully plastic and permanent [6]. However, our recently obtained experimental results suggest that the transient creep stage is actually composed of both viscoelastic and viscoplastic contributions. Based on this observation, we propose a new concept to model the rock salt mechanics specifically for hydrogen storage applications, which is based on incorporating both elastic and plastic deformations. More precisely, the proposed model utilizes the Kelvin-Voigt model [3] for the viscoelastic response and Perzyna's model with a non-associated flow rule [4] for the viscoplastic deformation. In addition, for the steady-state creep, pressure solution [10] and dislocation 1 creep deformations are both considered, as in our recent publication [8]. Finally, the accelerated creep stage is described by a damage evolution model [2]. The constitutive model is implemented in a finite element framework using the FEniCS package.

We show that this model is able to improve predictions of the salt rock mechanical behavior, using the laboratory experimental data as the benchmarking reference. Built on this new modeling approach, we investigate the impacts of the transient creep on the deformation of the salt cavern structures, in the presence of the heterogeneity and complex geometrical features.

Participation:

In-Person

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GROWTH OF BIOFILM AT PORE SCALE IN LAMINAR FLOW

Author: Araceli Martín[1]

[1] *UNIVERSIDAD POLITÉCNICA DE MADRID*

Corresponding Author: araceli.martin@upm.es

The Biofilm is a collective structure of microorganisms and it is covered by a protective layer secreted by the microorganisms themselves. The objective of this study is to identify and characterize the Elemental Biofilm Architectures that develop in a porous medium crossed by a laminar flow. This is a process that frequently occurs in nature, when there is water flow through the soil. In the

case of this study, a non-flagellated fluorescent mutant bacterium of P.Putida was used to analyze bacterial and biofilm growth through a homogeneous porous medium. In the experiments, different flow velocities and the percentage of nutrients (% LB Broth diluted in water) were tested. The results show different architectural formations such as streamers, chains, ripples and fine lines.

Two different methodologies were carried out during the experiments: Methodology A and B. With methodology A the bacteria were initially grown in the porous media, and then and bacterial free flow was injected at a constant flow rate. In methodology B, the porous media was initially free of bacteria, and a bacterial solution was injected at a constant flow rate during the experiment. With both methodologies, bacteria develop similar biofilm architectures, such as streamers and ripples; but distributed differently throughout the porous media. The biggest difference relies on the deposit profile: in Methodology A most of the biomass accumulates towards the outlet of the porous media, while for Methodology B towards the inlet.

Natural soils are home to an enormous variety of microorganisms. Microbial transport is important for a wide range of natural and artificial processes. However, the transport and distribution of bacteria in water flow at porous scale is still to be fully understood.

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MS09 / 854

Upscaling the rheology of non-Newtonian fluid flow in porous medium –a pore-scale study

Authors: Amna Al-Qenae[None]; Senyou An[1]; Rouhi Farajzadeh[2]; Vahid Niasar[3]

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The flow of non-Newtonian fluids in porous materials can be found in many industrial applications such as chemical engineering, subsurface engineering (de-contamination, energy production), and the food industry.

The relation between the shear stress and viscosity in non-Newtonian fluids is not linear and it is time-dependent, making it difficult to understand their behaviour. Due to the complex microstructure of pores in the porous media, the shear stress in each pore will be spatially variable, and thus the rheology of the non-Newtonian fluid would spatially vary along the flow pathways. Thus, it is very challenging to know how to upscale the shear-stress to estimate the upscaled porous

medium-based rheology. Experimental characterization of non-Newtonian fluid flow inside three-dimensional porous media is not feasible; however, pore-scale modelling offers a versatile tool to understand and simulate non-Newtonian fluid flow in porous media. The pore-scale modelling offers a better understanding of fluids rheology, viscosity, thermostability and flow diversion.

The present study examines the feasibility of upscaling the non-Newtonian shear-thinning fluid bulk rheology to porous medium rheology using the pore-network modelling approach. Laboratory work was done to obtain the fluid's bulk rheology. Then, a pore network model was constructed based on the Meter model equation and Hagen-Poiseuille law to simulate the porous medium rheology. The numerical results provided the pressure drop across the pore network for a given flow rate, fluids bulk rheology and pore-network geometrical and topological properties. As a result, the upscaled viscosity was back calculated using Darcy's law and compared to the bulk rheology. Due to the high cost and time consumption of the laboratory and modelling work, it is essential to find a simple way to predict the porous medium rheology from the bulk rheology. Thus, based on several simulation scenarios for various pore-size distributions, permeability and flow rates, an empirical equation was proposed to predict the porous medium rheology based on the bulk rheology and porous medium properties.

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Energy Transition Focused Abstracts:

MS01 / **855**

Caprock sealing capacity for underground hydrogen storage; Kimmeridge Clay

Author: Lubica Slabon[1]

Co-authors: Ian Molnar [1]; Katriona Edlmann [2]; Aliakbar Hassanpouryouzband [1]; Jennifer Roberts [3]

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Hydrogen for clean energy is in the national and international spotlight. Offshore wind presents an extensive renewable energy source in the UK, and a large green hydrogen resource, positioning the UK to be a major player in the emerging global hydrogen market. In the UK and around the globe there's a handful of likely subsurface hydrogen storage sites and it is widely recognised that hydrogen storage in porous media (rocks) will be necessary to support the scale of production, storage and use anticipated for a global hydrogen economy.
A key component of subsurface risk management is the suite of geological controls needed to ensure that storage is efficient and secure (i.e. that injected fluids do not leak from the storage formation).

Storage security is closely related to caprocks and their capacity to hold the stored hydrogen at the place for the needed period of time. The work characterizes and describes the Kimmeridge Clay. A caprock widely spread across the Central and Norther North Sea and which has acted as an effective seal for numerous hydrocarbon fields. Two key phenomena defining caprock ability to seal are capillary pressure (CP) threshold and displacement pressure (DP). Capillary pressure of the caprock needs to be sufficient to resist the upward buoyant forces of the hydrogen that is built up beneath the caprock and displacement pressure rules the flow of leaking hydrogen. Both capillary and displacement pressure are effected by pores/throats size distribution and wettability. The work focuses on porosity & wettability determination and an effect of these parameters on capillary pressure. The aims is to better understand caprock compatibility to hydrogen stored underground and to examine the processes conditional to caprock integrity and its sealing capacity.
Understanding of geological controls is critical to inform the selection of appropriate reservoir sites as well as designing safe and effective storage and recovery schemes. The work outcomes will inform (a) security, monitoring and assessment approaches for hydrogen geological storage, and (b) potential for engineered barriers for enhanced containment or leak remediation.

Participation:

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References:

Underground hydrogen storage

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MS11 / 856

Microscopic transport and phase behaviors of CO2 injection in heterogeneous formations using microfluidics

Authors: Yaohao Guo[1]; Zhi Xu[2]; Bo Bao[2]

[1] *East China University of Science and Technology; University of Toronto*

[2] *East China University of Science and Technology*

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CO2 injection into the geological formations is a promising option to enhance oil recovery while simultaneously contributing to carbon storage. Conventional core tests provide critical insights but still leave ambiguous transport mechanisms due to the limitation of real-time visualization. This study aims to directly observe the multiphase flow behaviors and phase change in CO2 injection at pore-scale using microfluidics. Our all-in-one chip design provides a universal platform to reproduce various CO2 injection strategies in the formation with permeability contrast, including flooding and huff-n-puff processes, and integrated a rapid measurement of minimum miscibility pressure (MMP). Miscible injection eliminates the capillary force in immiscible scenario, and promotes stable film-wise displacement with a higher recovery rate and an attenuated heterogeneity impact. We find that effective huff-n-puff operations require a sufficient gas concentration to generate bubbles and an adequate pressure gradient to push the dissolved gas displacement, which supports the importance

of high depressurization rate from both physical phenomenon and inherent mechanism. Huff-n-puff re-energizes the reservoir after immiscible flooding through deep gas-oil interactions and induces a considerable growth in cumulative recovery. These micromodel results can significantly improve our fundamental understanding on detailed multiphase transport phenomena in CO2 injection and help to optimize implementation schemes.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 857

Comparative study of hydrogen and CO2 performance in subsurface using sharp-interface modelling

Authors: Ehsan Vahabzadeh Asbaghi[1]; Vahid Niasar[1]

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The increasing need for hydrogen storage on a large scale has motivated new ideas on different methods of underground storage. Saline aquifers may offer a practical option for hydrogen storage due to their geographic availability and large capacity. However, reservoir engineering aspects of the injection and withdrawal of hydrogen in aquifers are yet to be understood. While 3D reservoir simulations offer rigorous but they are computationally demanding. Alternatively, sharp-interface models can be implemented to still get an accurate description of fluid flow in the porous medium and have less complexity compared to widely-used 3D simulators.
Sharp-interface models are based on the vertical equilibrium concept that considers the presence of a sharp interface between two phases due to the significant density difference between brine and gas and can be applied to reservoirs with a high aspect ratio that makes the vertical fluid flow negligible compared to horizontal flow. The sharp-interface model is widely utilized to study CO2 injection in saline aquifers, so it can also be valid for hydrogen and brine systems, as hydrogen is much lighter than CO2.
In this study, the sharp-interface model from MRST-co2lab is utilized to simulate hydrogen storage in the Johansen formation. The Johansen saline aquifer is one of the large-scale CO2 storage prospects that also have the criteria of the vertical equilibrium approach. This study aims to understand how the difference in densities and viscosities between CO2 and H2 impacts the performance of storage and withdrawal efficiency. For this purpose, CO2 and H2 are injected and withdrawn for four cycles under similar operational conditions and reservoir properties. As CO2 has a higher density and viscosity, its concentration would be higher in areas close to the wellbore, but the hydrogen spreads widely throughout the reservoir. Additionally, the storage ability of H2 is lower than CO2 due to its higher gravity override, though its withdrawal ability is higher than CO2.

Participation:

In-Person

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MS05 / **858**

Influence of mineralogy on Sporosarcina pasteurii attachment in engineered and natural porous media

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[1] *The University of Michigan*

[2] *University of Michigan*

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Microbially-induced carbonate precipitation (MICP) has demonstrated promise in a variety of subsurface applications including immobilization of groundwater contaminants and remediation of leakage pathways associated with CO2 sequestration. In order to implement MICP at the field scale, however, the injection strategy must be tailored for efficacy in natural, heterogeneous porous media. Specifically, the overlapping effects of varied mineralogy and pore geometry on bacterial attachment, growth, and mineralization must be fully resolved. While the affinity of microorganisms for certain minerals (e.g. carbonates and clays) over others (e.g. silicates) is established, and biomass growth rate is known to be mediated by variables such as pH, such insights must be synthesized to develop injection strategies that produce desirable quantities and distributions of precipitate.

In this study, we investigate four questions pertaining to the influence of mineralogy on final precipitate distribution in a typical MICP injection consisting of separate attachment, growth, and mineralization phases. First, we assess to what extent initial biomass distribution is correlated with mineralogy. To this end, we construct modular columns to resolve average attachment rate versus distance from inlet; attachment rates are then determined experimentally for a set of common minerals including silica sand, kaolinite, Na-montmorillonite, and natural limestone grains, with parameters including grain size distribution, flow rate, and pH held constant. Second, we examine the correlation between final precipitate distribution and initial biomass distribution; this is accomplished by post-MICP characterization of columns via X-ray computed microtomography (XCT) for spatially-resolved precipitate distribution. Third, we attempt to decouple final precipitate distribution from initial biomass distribution through two modifications to the growth stage of injection. These include mechanical redistribution of biomass through rapid flow-induced shear sloughing, and slowing of biomass growth rate near the inlet via influent media acidification. Finally, we determine whether these modifications remain effective when applied to natural cores of clay-rich sandstone,

whose pore size distribution differs from the engineered columns. Taken together, these experimental results elucidate the influence of mineralogy on the distribution of precipitates for typical MICP processes, and suggest avenues for optimizing injection strategy given mineralogy.

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In-Person

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Energy Transition Focused Abstracts:

MS13 / **859**

Temperature-Dependent Behavior of Bicontinuous Microemulsions in Pores

Author: René Haverkamp[None]

Co-authors: Margarethe Dahl [1]; Stefan Wellert [1]; Thomas Hellweg [2]

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Microemulsions are thermodynamically stable solutions composed of water, oil, and amphiphilic components such as a surfactant. They show a fascinating variety of structures and properties that have been explored over the past few decades. Numerous applications in areas such as pharmaceuticals, cosmetics, enhanced oil recovery, the food industry and many more make the relevance of this research clear 1. The properties of microemulsions in porous materials are relevant for many of these applications. In our work we therefore focus on the sponge phase of a ternary microemulsion based on a surfactant of the type CE in controlled porous glasses (CPG) as a model system. CE Surfactant-based microemulsions are well-characterized model systems, and the porous material CPG is available in a variety of pore sizes. Preliminary work on the behavior of this microemulsion at planar glass interfaces showed a structure-directing influence of the glass surface, which led to a lamellar structure near the interface, which gradually transformed into the sponge structure in the volume phase with increasing distance from the glass surface [2]. This effect is present in both hydrophilic and hydrophobic interfaces. [3] To study the structural changes within the pores, we use small-angle X-ray/neutron scattering (SAXS/SANS). By measuring the temperature-dependent phase behavior of the microemulsion in the pores compared to the temperature-dependent phase behavior in the bulk with SAXS, we have already obtained detailed information about the effects of confinement on the structure. This was accomplished by measuring the correlation length of the microemulsion in the pores, which is indicative of the size of the microemulsion droplets. For pore diameters from 1000 nm to 240 nm in the temperature range from 5 to 55 ℃ we observe a behavior similar to that in the bulk phase. At low temperatures, where the main microemulsion would consist of two separate phases, the microemulsion droplets are small. With increasing temperature, the curvature of the droplet interface decreases, resulting in larger droplets overall. After reaching the zero curvature limit, a further increase in temperature leads to inverse droplets that become smaller with increasing temperature. For small pore diameters of 184 nm we observe the same size over the

entire temperature range. Overall, we observed a high influence of the pore walls at small pore diameters. Based on these results, experiments with the contrast matching SANS method are planned to get more information about the actual structure of the microemulsion in the pores.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS09 / 860

Development of a thermodynamically-based pore-scale network model to simulate fluid intermittency during two-phase flow.

Authors: Ademola Adebimpe[None]; Martin Blunt[1]; Branko Bijeljic[2]; Sajjad Foroughi[3]

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We developed a thermodynamically-based pore network model to simulate fluid intermittency during two-phase flow through porous media. Relationship between pressure gradient and flow rate during multiphase flow in porous media have been observed to transition from linear to non-linear at intermediate flow rates in recent studies. With the aid of high resolution X-ray tomography, intermittent filling of the pore spaces by the phases has been observed resulting in a nonlinear relationship between the pressure gradient and flow rate. Existing pore network models have not been able to reproduce this phenomenon. We first develop a quasi-static pore-network model to simulate the drainage and imbibition processes where capillary forces dominate. We then modify this quasi-static model by introducing a probability distribution of filling inspired by the thermodynamic formulation of multiphase flow proposed by Hansen and colleagues. The probability distribution is formulated by drawing an analogy between thermodynamics and fluid flow in porous media. We have shown that a simple thermodynamically-based pore network model can simulate the nonlinear intermittent fluid behaviours during two-phase flow through porous media.

Participation:

In-Person

References:

Hansen, A., Flekkoy, E.G., Sinha, S. and Slotte, P.A. (2022). A Statistical Mechanics for Immiscible and Incompressible two-phase Flow in Porous Media.

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MS06-B / 861

Singularities and surprises in porous media models of interfacial non-Newtonian flows

Author: Prabir Daripa[1]

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We consider the Hele-Shaw model of porous media flows involving two immiscible upper convected Maxwell fluids [1, 2]. Linear stability analysis shows that singularities up to three types can occur including resonance and fracture, the latter one consistent with the experimental results of Mora and Manna [3]. The resonance occurs when one of these two fluids is air and is removed when air is replaced by a Newtonian fluid. The Oldroyd-B case currently in progress will also be discussed. This is joint work with Zhiying Hai.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 862

Geometric Characterizations for the Prediction of Electrical Properties in Porous Media

Author: Bernard Chang[1]

Co-authors: Rodolfo Victor [2]; Masa Prodanovic [1]

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Electrical transport properties through porous media have widespread applications in reservoir formation evaluation, groundwater management, mineral exploration, and carbon capture and storage (CCUS) monitoring. Additionally, advancements in 3D imaging and computing have enabled unprecedented visualization and analysis of these pore scale processes. However, relationships between a porous medium and its electrical properties are typically reported in terms of volume-averaged variables, such as porosity and fluid saturation. The contributions of the local geometries are not readily interpretable, making it difficult to generalize models to heterogeneous mediums and to larger scales.

Here we present a statistical study to provide insight into the local geometric descriptors of the conductive phase that best characterize electrical transport properties. The study consists of a similar workflow used in feature engineering and selection for data-driven machine learning models. The data used in this study has been published on Digital Rocks Portal and is, to our knowledge, the most extensive set of standardized, open-source simulations in heterogeneous porous media images. We further extend these geometric descriptors to be used as input features into a convolutional neural network architecture to predict the electric current field. The results of this study can improve the interpretability and training efficiency of machine learning models and help categorize porous media systems for prediction of macroscopic properties. They also provide useful insight for understanding electrical behavior through complex porous media.

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Energy Transition Focused Abstracts:

863

Multi-scale investigation of pressure drop and heat transfer coefficient in packed beds at high temperature

Author: Shaolin Liu[None]

Co-authors: Azita Ahmadi-Senichault [1]; Hermes Scandelli ; Jérémy Chevalier [2]; Jean Lachaud [3]

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Fixed beds of randomly packed particles have been used for decades in chemical engineering. Thermal energy storage in packed beds is receiving increased attention as part of energy transition efforts. A proper understanding of the mechanisms of heat transfer and pressure drop through packed beds are important for the design of high temperature energy storage systems. Because energy transfer is related to many parameters such as void fraction, particle size, fluid velocity and solid thermal conductivity, it is necessary to understand the influence of these parameters on the system behavior. In this work, we investigated the pressure drop and heat transfer coefficient within a randomly packed bed using a multi-scale approach,that relies on simulations at the micro-scale, the macro-scale, and experimental measurements. For the simulations at the micro-scale, a 3D model of a randomly packed bed filled with spheres was generated using the open-source software LIGGGHTS1. Numerical tools based on OpenFOAM were used to mesh the geometry and solve the Navier-Stokes equations and heat transfer equations in the fluid and solid domains respectively. An integral method [2] was used to compute the heat transfer coefficient. It is calculated as the ratio of the heat flux at the solid-fluid interface and the difference between the averaged temperatures of the two phases. For the simulations at the macro-scale, a 2D axisymmetric geometry was generated to represent the 3D model. PATO [3] was used to solve Darcy-Forchheimer's flow and local thermal no equilibrium equations (LTNE) inside packed beds. The heat transfer coefficient and effective gas thermal conductivity tensor were obtained from the simulations. In parallel, an experiment consisting of hot gas flowing through a packed bed filled with glass beads was performed [4]. The evolution of the pressure gradient with the Reynolds number was calculated based on the experimental results. The heat transfer coefficients obtained by an inverse analysis method [4] were compared with the results obtained by the integral method. The results showed that the permeability and the Forchheimer coefficient were respectively $2.95\times10^{-7}m^2$, and $1.037\times10^{3}m^{-1}$ in the simulations on the micro-scale. These two values are $9.44\times10^{-8}m^2$ and $6.57\times10^{2}m^{-1}$ in the experimental results. The maximum relative error on the resulting pressure drop is 35%. The heat transfer coefficient increases from 8450 $W/(m^3\cdot K)$ to 11700 $W/(m^3\cdot K)$ during the 3000s of the micro-scale simulation and it increases from $10010W/(m^3\cdot K)$ to $11900W/(m^3\cdot K)$ during the experiment. The maximum relative error between the heat transfer coefficients is 18%. Besides, the simulation results obtained at the micro scale show that the heat transfer coefficient is a function of time and thermal properties. It increases as Biot number decreases for a given gas velocity. This work connects simulations at the micro-scale, macro-scale, and experimental measurements. The comparison shows that additional work is needed to lead a perfect argument. However it provides interesting insight and opens possibility to study pressure drop and heat transfer coefficients from a multi-scale perspective.

Participation:

Online

References:

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865

Enhancement of the longitudinal modulus of liquid adsorbates in nanoporous Vycor glass

Authors: Klaus Schappert[1]; Rolf Pelster[1]

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Nanoconfinement changes the elastic properties of adsorbates and causes deviations from the bulk properties [1,2]. The size of the nanopores is a major factor influencing the elastic moduli of adsorbates 1. Intriguingly, ultrasonic experiments with the adsorbates argon and nitrogen in nanoporous Vycor glass revealed for these two adsorbates significant differences in the magnitude of the enhancement of both the longitudinal modulus and the shear modulus [2,3]. Here we study the enhancement of the longitudinal modulus of different liquid adsorbates in nanoporous Vycor glass using ultrasonic measurements. We discuss the influences of the interaction strength between adsorbates and the pore surface and other factors on the modulus of the adsorbates.

Participation:

Online

References:

1 Christopher D. Dobrzanski, Boris Gurevich, and Gennady Y. Gor, Elastic properties of confined fluids from molecular modeling to ultrasonic experiments on porous solids, Appl. Phys. Rev. 8, 021317 (2021).
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Energy Transition Focused Abstracts:

Poster / 867

Mediation of water vapour transport in nanopores via salt solutions: thermodynamic and kinetic study

Author: Sujeet Dutta[1]

Co-authors: HUGO BELLEZZA ; joachim trosseille ; Alexandre Littiere [2]; Patrick Huber [3]; Olivier Vincent [4]

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[2] *Ecole normale supérieure Paris-Saclay*

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Volumetric water vapour sorption isotherms have been carried out in nanoporous monolithic glass membranes (Vycor) in both empty and salt solution (Li-/NaCl) filled pores in order to investigate the relative humidity and pore-filling fraction associated with capillary condensation and peak desorption/desorption-tension, and the impact of salt solution activity/chemical nature on such processes. Subsequently, optical reflectance (imaging) measurements have been
conducted on the same systems (Vycor membranes filled with different salt solutions) using a home-made controlled environment (temperature and relative humidity under vacuum) setup in order to identify the thermodynamic signatures of specific processes, such as adsorption/desorption tension activity, formation of salt solution clusters, and crystallisation. The correlation between the volumetric and optical experiments have been investigated to unravel the pore filling/emptying mechanisms, and the role played by salt ions in mediating the transport of water molecules. The results of this analysis have been compared to the ones obtained from molecular dynamics simulations of desorption of salt solutions from an interconnected pore network . Ongoing studies reveal a second order transition from vapour to condensed liquid filled pores for salt solutions, contrary to a clearly defined first order capillary condensation observed for empty pores. Results also indicate that the salt solution clusters develop within the pores during the desorption process strongly retard the escape of water molecules, causing the desorption process to spread over a wide humidity range. Further thermodynamic treatment of the sorption isotherms help attain a clearer understanding of the associated pore-emptying mechanisms, such as homogeneous meniscus recession/cavitation/pore-blocking under a simultaneously occurring ionic-rearrangement of the salt along the pore walls. The next step involved investigating the kinetics of vapour phase imbibition of nanoporous membranes filled with salt solutions, followed by drying once the pore filling reached saturation. In such experiments, the Vycor membranes were sealed on all sides, except one left free for transport of water molecules. This led to a 1D imbibition/drying front, the progress of which could be plotted against time for its analysis by appropriate kinetic models. Preliminary analysis suggests that both wetting and drying processes are significantly retarded when salt is present inside the nanopores. Results also indicate that the drying kinetics is strongly governed by the activity of the confined salt solution, as a dynamically developing humidity gradient along the length of membrane may lead to a gradient in the salt percolation network. At present, evaporation of water from isolated horizontal nanochannels filled with salt solutions is being investigated, which may be connected to vertical nanopores in future studies (in a different nanofluidic device) to quantify the mass transport of water from a single model pore geometry and the impact of salt solution activity/chemical nature on it.

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MS02 / 869

A hydrogel-soil system to enhance plant water uptake

Author: Pooria Ghadir[1]

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By 2030, a third of the population in developing countries will reside in areas where the gap between water demand and supply is predicted to be over 50%. Agriculture is responsible for over 71% of annual water withdrawals worldwide (currently ~ 3,100 billion m3 and predicted to be ~4,500 billion m3 by 2050). The amount of water held as groundwater is more than 100 times the amount collected in rivers and lakes. Globally, the per capita irrigated area has been decreasing for 30 years. Population growth and increased irrigation requirements have resulted in groundwater mining with a universal increase in water table depth.
A preliminary study aimed at developing a bioinspired pump capable of passively lifting subsurface water is presented. The bioinspired system uses emerging materials and concepts in geotechnical engineering to mimic the wicking mechanisms that plants use for transpiration. Upon droughts and dry periods, soil desaturates, its hydraulic conductivity drops and less water is made available to plants. As water inflow to the plant decreases, stomata close to stop transpiration and prevent plant dehydration, photosynthesis ceases, and plants wilt. Upon dry conditions, to delay soil desaturation, preserve a high hydraulic transmissivity and extract water for longer, plants secrete a gelatinous substance named mucilage around root tips. This naturally engineered "grout"fills the pore space by reducing the pore diameter and increasing the soil air-entry value (creating smaller capillaries).
A capillary network aimed at mimicking plant mucilage secretion is formed by the injection of colloidal silica-based hydrogel (CS) into the soil. It is shown that the presence of hydrogel enhances soil hydraulic conductivity and water retention capacity thus enabling better water uptake during periods of drought. A hydromechanical characterization of the hydrogel-soil system and preliminary experimental results of the hydrogel interaction with the roots of various species of shrubs will be presented.
Keywords: Colloidal silica hydrogel; plants; drought; capillary rise; roots

Participation:

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Energy Transition Focused Abstracts:

MS01 / 870

Microfluidic Study of CO2 Dissolution Dynamics under Geological Sequestration Conditions

Authors: Wei Yu[1]; Jack H.Y. Lo[1]; Xianmin Zhou[1]

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CO2 geologic sequestration in deep saline aquifers and depleted oil reservoirs is an effective option for large-scale and long-term carbon mitigation to address global climate challenges.1 After being injected into the target geological formations with a low permeability caprock above them (structural trapping), CO2 is stored by trapping in the pores (residual trapping), dissolving in the formation water (solubility trapping), and reacting with the minerals (mineral trapping).[2] Solubility trapping is significant both in the amount of trapping capacity they provide and long-term storage security in the long term (>100 years).[3] In addition, the transformation of CO2 from a separate phase to CO2 (aq) and HCO3- by dissolution will influence the mineral dissolution and precipitation processes, which is critical to permanent carbon storage.[4]

In this work, we studied the CO2 dissolution dynamics in porous media under realistic reservoir conditions of deep saline aquifers. We developed a high-pressure and high-temperature microfluidic system and captured the spatio-temporal evolution of the dissolution process of residual trapped CO2 under various pressures and temperatures (gas, liquid, and supercritical CO2). The CO2 dissolution kinetics was calculated by analyzing the optical images obtained by a high-resolution camera. The results showed a two-stage process of CO2 dissolution into the aqueous phase in porous media. In the first stage, CO2 dissolves rapidly into the ambient aqueous phase to reach a local saturation. The second stage showed a lower but constant CO2 dissolution rate with the CO2-water interface propagating linearly with time toward the CO2 phase. The CO2 dissolution rate is sensitive to the sequestration pressure and temperature, whereas supercritical CO2 shows a more than ten-time slower dissolution rate than gaseous CO2. Moreover, dissolution-induced fingering of water invading CO2 was observed due to local pressure instability, which would affect the two-phase flow of CO2 and the formation water. Our research reveals the CO2 dissolution mechanisms in porous media under geological sequestration conditions, which provides a new insight for estimating the time scale for CO2 geological sequestration.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / **871**

Trapping, Hysteresis and Ostwald Ripening in Hydrogen Storage: A Pore-Scale Imaging Study

Authors: Sepideh Goodarzi[None]; Yihuai Zhang[1]; Guanglei Zhang[2]; Branko Bijeljic[2]; Martin Blunt[3]

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Gas injection and withdrawal in the subsurface can be considered as a long-term energy storage solution. Green gas can be produced from the excess electricity during peak production and can subsequently be injected into the surface reservoir and withdrawn during times of high demand. Repeated injection and withdrawal of gas causes capillary pressure hysteresis –in this work we use X-ray tomography to understand the hysteresis phenomenon, which can be applied in operating underground hydrogen storage processes. Two experiments were performed at an unsteady state to investigate gas and water distribution in different pore space geometries during drainage and imbibition cycles. Gas phase was injected into 6 cm long samples of Bentheimer sandstone and Estaillades carbonate at ambient temperature and a pore pressure of 1 MPa, followed by water flooding in three cycles. The gas flow rates decreased from 2 ml/min to 0.08 ml/min while the brine injection rate was keeping constant during the three cycles. We observe and quantify several interesting phenomena including (I) capillary pressure hysteresis, and (ii) hydrogen migration by Ostwald ripening through diffusion of gas dissolved in the brine. We characterise these phenomena by analysing interfacial curvature and area, along with wettability and pore occupancy analysis. This work provides pore-scale insights into hydrogen storage and withdrawal and uses image-based analysis to quantify multiphase flow properties for input into the reservoir-scale simulation.

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MS10 / **873**

Analysing salt precipitation-damage coupling in limestone with 4D X-ray tomographic imaging

Author: Syrine BEN ELHADJ HAMIDA[None]

Co-authors: Marijn Boone [1]; Veerle Cnudde [2]; Peter Moonen [3]; Hannelore Derluyn [4]

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Climate change leads to intensified weathering cycles on landscapes and the built environment. Energy transition strategies such as seasonal storage of biogas or hydrogen in aquifers, introduce cyclic perturbations in the underground environment. In both cases precipitation-dissolution cycles of salts are induced. When precipitation occurs inside the pore space, stresses build up which may eventually crack the material. This might lead to severe deterioration of natural stones, as present in our historic monuments or natural landscapes. In addition, precipitation-dissolution of salts as well as crystallization-induced cracking alter key petrophysical properties of the rock matrix itself, such as its permeability, thus impacting gas injectivity.
Understanding the exact coupling between transport, salt precipitation, crack initiation and propagation in natural porous media remains an open research subject. Experiments in which transport, precipitation and fracture kinetics can be studied simultaneously are essential to advance our insights in these coupled phenomena. To that extent, a 4D micro-tomographic dataset has been analyzed of a Savonnières limestone plug subjected to NaCl precipitation and dissolution. The sample consists of two zones with different wettability, i.e. a hydrophobic and a hydrophilic part, and is initially saturated with a brine solution. Precipitation is induced by drying the sample via the hydrophobized part, creating crystallization-induced fractures at the hydrophobic-hydrophilic interface. Dissolution occurs by subsequently exposing the sample to a highly humid environment, above the deliquescence point of NaCl, which leads to a rewetting of the sample and a dissolution of the salt crystals, as well as a partial closure of the fractures. The sample is imaged at a 9 μm voxel size, every 30 minutes during the first day of drying, and every hour during the second day of drying and the third day of deliquescence. The image processing consists, in a first step, of a global analysis using a customized Python script, allowing to extract information on porosity and pore size changes, the crystal deposition in the pores, and the global deformation of the sample. In a second step, digital volume correlation, using the SPAM software (Stamati et al. 2020), is employed to determine the local displacement fields, and thus the local strain, on the 3D volume of the deforming sample. The spatial and temporal resolution of the acquired dataset, combined with the developed image analysis workflow, allows to highlight the coupling between the stone's pore structure, precipitation/dissolution and fracture kinetics, at the pore scale level. These experimental observations then assist in refining existing poromechanical models of in-pore salt crystallization and crystallization-induced damage.

Participation:

In-Person

References:

Stamati et al., (2020). spam: Software for Practical Analysis of Materials. Journal of Open Source Software, 5(51), 2286, https://doi.org/10.21105/joss.02286

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Energy Transition Focused Abstracts:

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874

Unravelling Dynamic Wetting Behaviour Inside Sponges for Oil/Water Separation

Authors: Pavani Cherukupally[1]; Gijs Wensink[2]; Veerle Cnudde[3]; Laurenz Schröer[3]; Maja Rücker[2]

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Separating toxic organic pollutants from wastewater is a significant environmental challenge for remediating petrochemical industrial effluents 1 and cleaning accidental oil spills [2,3]. Surface-engineered sponges (SEnS) have emerged as a possible solution due to their low cost, easy manufacturing, simplicity to reuse, and ultrahigh performance. Previous studies reported SEnS with critical surface energy achieved by coating porous polymeric sponges with long-chain alkanes capped nanosilica for removing over 99% of the crude oil pollutants from the wastewater within 10 minutes [1,2,3].

Next, to implement the SEnS as a separation media in industrial-scale filtration devices, the structural parameters, such as surface composition and/or size of the pores, multiphase flow patterns, and velocities, needs to be optimized. However, to our knowledge, no studies evaluated dynamic wetting or multiphase flow behavior inside the SEnS in the context of oil/water separation. Alternatively, multiphase flow in geological systems, such as rocks, correlated surface chemical and structural attributes of the porous medium with variable flow patterns have been reported previously [4]. In this study, inspired by the dynamic wetting studies inside the porous rocks, we aimed to investigate how flow patterns manifest within the sponge's pores and how surface modification effect those.

In this work, the dynamic wetting behavior inside sponges was performed on unmodified polyurethane sponges, modified with alkyl, aminiosilane, and alkyl-aminiosilane surface functional groups. The spontaneous imbibition of bulk oil into the four candidate sponges was imagined by pre-wetting them with brine or saline water. In addition, we submerged the sponge into emulsified oil/water mixture and imaged the evolution of the wetting phenomenon to reflect the petrochemical wastewater in real-world conditions. We obtained the images with the CT-scanners, Environmental Micro-CT (EMCT) [5], and TESCAN CoreTom, at the University of Ghent.

The CT images of the bulk oil and brine wetting showed a minor difference in fluid reconfiguration at the resolved pore scale. However, upon application of contrast, we noticed fluid exchange in the non-resolved nanostructure of the sponge fibers. Similarly, for the oil/water emulsions system, nano-scale fibers showed the onset of dynamic wetting and multiphase flow evolutions. After the sponge fibers adsorb the oil, these fibers facilitate the formation of larger drops that adhere to the sponge surface. These results confirm that surface wetting of the nano-scale fibers, but not the pore filling, is the main mechanism of emulsified and bulk oil adsorption onto the SEnS. In the future, these insights into the physical adsorption phenomenon will be used to optimize the surface design of the sponges and flow properties for practical sponge-based oil/water separation systems.

Acknowledgments: This work is sponsored by the Excite Network (European Union's Horizon 2020 research and innovation program, grant agreement No 101005611), Global Challenges Reserach Fund by the UK Research and Innovation, and Banting Postdoctoral Fellowship by the Canadian Institutes of Health Research.

Participation:

Online

References:

1 Cherukupally et al. (2020). Surface-engineered sponges for recovery of crude oil microdroplets from wastewater. Nature Sustainability, 3(2), 136-143.
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MS09 / **875**

Multi-scale pore network model for simulation of multi-phase flow in heterogeneous porous media

Author: Sajjad Foroughi[1]

Co-authors: Branko Bijeljic [2]; Martin Blunt [3]

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Pore network modelling as a robust and powerful technique has been used to study multiphase flow through porous media for many years. Micro-CT imaging makes it possible to acquire actual pore structure geometry used to extract the pore network structure. Also, multiphase micro-CT images can be used to calibrate the pore-scale distribution of wettability. However, in many kinds of porous media both in nature and industry, the pore size distribution covers many orders of magnitude in length scales where it is not possible to resolve all the pore space in a single image. For example, micron-resolution imaging of a sample a few mm to cm across cannot explicitly resolve sub-micron porosity which may have a significant impact on flow behaviour. Therefore, considering sub-resolution pore space in pore network modelling is necessary.

Experimentally, differential micro-CT imaging, comparing a dry image with an image of a sample completely saturated with a contrast fluid (usually a high-concentration brine) allows porosity to be quantified voxel-by-voxel. In this study, we have developed a workflow to incorporate unresolved porosity in our modelling. For this purpose, wherever the micro-porous region (with a voxel porosity less than 1 but greater than zero) connects to resolved pore space (voxel porosity of 1) a micro-link is considered. An automatic parallelized algorithm helps to identify micro-links incorporated in the pore network extracted from resolved pores. While resolved pores are treated similarly

to a conventional pore network model, the micro-links are treated as continuum Darcy-type porous media in which empirical correlation are be used to determine their parameters. Due to the uncertain nature of the unresolved pore space, we tune the parameter of the empirical models to match observed experimental behaviour, such as permeability and primary drainage capillary pressure, using a multiscale pore network model. Finally, we applied this workflow to model multiphase flow in Estaillades limestone and a complex reservoir rock sample in which more than 50% of the pore space is unresolved in our micro-CT images, and simulation using multi-scale model is necessary.

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Energy Transition Focused Abstracts:

MS06-A / 876

Capillary entry pressure in soft porous media

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[1] *University of Oxford*

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The capillary entry pressure is a fundamental quantitative parameter in two phase flows in porous media. The entry pressure is set primarily by the interfacial tension between the invading and defending fluids, the relative wetting properties of the fluids on the solid skeleton, and the length scale of the pore throats. In rigid porous media, all of these quantities are typically fixed, meaning the entry pressure is a constant for a particular choice of medium or fluids.

Here, we consider entry pressure for very soft porous media: specifically, those with elastic moduli comparable to the characteristic capillary pressure scale of the system. In such media, the pore geometry may undergo significant deformations due to the injection of an invading phase. As a consequence, the size of the pore throats and, hence, the entry pressure may evolve dynamically. We investigate how entry pressure is impacted by deformation using an idealised model experimental system comprising a quasi-2D column of water-saturated hydrogel beads, which we compress using a "capillary piston": a pressure-controlled bubble of non-wetting gas that squashes the column along its length, driving liquid from the far end of the column via a permeable barrier. These experiments are complemented with simple analytical models of analogous systems.

We begin by considering quasistatic loading and then extend our study to rapid dynamical loading. The latter scenario introduces a viscous pore pressure, which further opposes the entry of gas into the pore space. We discuss how the transient consolidation flow driven by the capillary piston introduces a spatial distribution of pore and solid stresses and, hence, a spatially-distributed capillary entry pressure within the system. We consider how we may decouple the different forces at work to extract quantitative knowledge of deformation-dependent entry pressure from experimental observations of percolation in soft porous media.

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Energy Transition Focused Abstracts:

MS21 / 877

Measuring the changes in the pore size distribution of a soil sample during its compression using non-Newtonian fluids.

Authors: Martin Lanzendörfer[1]; Soheil Safari Anarkouli[1]; Martin Slavík[1]; Tomáš Weiss[1]; Jan Najser[1]; Jakub Roháč[2]

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While there are many methods available for the characterization of pore sizes of soils and other geological materials, most of them are expensive or destructive or, in fact, both. Non-Newtonian fluids have been utilized recently for that purpose, providing not only a cheaper and more accessible alternative to the classical porosimetry techniques but also a method that does not disturb the sample and can be used repeatedly. In particular, the so-called ANA method 1 derives the effective pore size distributions of the porous sample based on a set of saturated flow experiments with different shear-thinning fluids, in our case the aqueous xanthan gum solutions of different concentrations.

We will discuss a methodology to measure the progressive changes in the pore size distribution of a sample of sand that is placed in the standard triaxial test chamber and subject to a drained compression. After every compression step (i.e. after increasing the pressure level maintained in the chamber, thus further compressing the sample), a sequence of permeability measurements with fluids of different rheology is performed and the effective pore size distribution is approximated. The ANA approach is used in our case since the similar yield-stress method [2] requires using larger hydraulic gradients, which would disturb the effective stress imposed on the compressed sample.

1 Hauswirth, S.C., Abou Najm, M.R., Miller, C.T., 2019. Characterization of the Pore Structure of Porous Media Using non-Newtonian Fluids. Water Resources Research 55, 7182–7195. https://doi.org/10.1029/2019WR025044

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Poster / 878

Freezing and Thawing Process in Porous Media: A Study Using Magnetic Resonance Imaging and Modeling

Authors: Michal Snehota[1]; Andreas Pohlmeier[2]; Martina Sobotkova[3]; Tomas Princ[4]; Michal Benes[5]; Martin Jex[5]

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Freezing and thawing of water in porous media depend on pore size distribution and shape of particles. Magnetic resonance imaging (MRI) of the freezing and thawing process was performed on two samples of different porous materials, each one in two replicates. The experiment was subsequently numerically simulated. The set-up consisted of a double-walled Plexiglas container. The inner cylindrical container (3 cm inner diameter, 6 cm high) was filled with the sample material. On the top of the porous media, a glass disk (2.8 cm in diameter, 1 cm thickness) was placed to define the upper boundary of the material during freezing and thawing. One inflow tube and two outflow tubes at the top of the inner cylinder were used for the circulation of cold nitrogen gas as a freezing medium to the top of the sample. The temperatures of the freezing medium were continuously recorded by the temperature sensors located outside of the MR coil. The first sample packing consisted of 72 glass beads, 0.8 cm in diameter immersed in the 1 mM/L GdDTPa2-·2Na+. In the second sample, the coarse sand was packed in 0.5 cm thick layers in the same sample solute. A total of eight freezing-thawing cycles were performed and recorded on the samples. As a result, time-lapse series of 3D MR images were obtained. The analyses of the freezing-thawing process on glass beads revealed interesting effects while thawing, where the thin layers on the glass beads surface exhibited faster melting in otherwise homogeneous ice. The freezing-thawing fronts recorded of sand samples were relatively uniform. The spatiotemporal analysis of the frozen water volume is done.
Numerical simulation of the observed phenomena is performed by the model based on the conservation of mass, energy, and momentum solved by the finite-element method. The model provides information on the distribution of temperature, both phases and on structural changes in the porous structure caused by the phase transition. The model serves for better understanding of observed phenomena and optimization of the experiments.

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Energy Transition Focused Abstracts:

MS03 / **879**

Elastic normal fracture deformation in thermoporomechanical media

Author: Ivar Stefansson[1]

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Many subsurface processes feature mechanically closed fractures elastically deforming in response to stress changes. In cases involving temperature contrasts, such as geothermal reservoirs, these changes are typically due to thermal stresses as well as pore pressure. In turn, changes in hydraulic fracture apertures impact the flow field and thereby also heat transport, resulting in a strongly coupled system of governing equations. We study this interplay drawing on a series of numerical simulations using the fracture simulation toolbox PorePy. The thermoporomechanical system is solved fully coupled in both fractures and matrix, ensuring a rigorous numerical representation of the modelled processes.

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MS06-A / **880**

Effects of molecular details on two-phase flows through nanopores

Authors: Petter Johansson[1]; Guillaume Galliero[2]; Romain Vermorel[3]

[1] *LFCR, Université de Pau et des Pays de l'Adour*

[2] *LFCR, E2S-UPPA, Université de Pau et des Pays de l'Adour, France*

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Geological storage of carbon dioxide and spent nuclear fuel are topics of huge significance for our societies. This motivates an improved understanding of fluid transport of gases through partially saturated porous networks such as clay materials or caprock. However, this is a complicated problem spanning length scales from nano- to millimeter sized channels. To fully model drying, evaporation and diffusion through these networks we need to understand the dominating physics at all scales. At nanometer scales the molecular nature of fluids becomes apparent. For multiphase fluid systems this involves fluid–fluid interfaces, which have explicit widths of several molecules across and physical properties separate to those of the bulk phases. Physical modeling of multiphase flows must include these effects when applied to systems of sizes approaching the nanoscale 1.

We present our work on resolving these molecular details of fluid–fluid interfaces in two-phase systems. Since it is inherently difficult to study nanoscale behavior in laboratory experiments, our approach is by the use of molecular dynamics (MD) simulations of gas/liquid flows through nanopores. MD simulations are fully atomistic and so include realistic molecular effects by its nature. However, molecular simulations of multiphase flows at the nanoscale are still challenging and should be achieved with care and adequate methodology, as proposed in this work, to avoid unphysical behavior. These numerical experiments give us physical insight in how molecular interfaces affect two-phase flows in nanochannels. We also show how these effects can be included as effective quantities or boundary conditions in continuum physical models of similar systems.

Participation:

In-Person

References:

1 Johansson, Galliero, Legendre. How molecular effects affect solutal Marangoni flows. Physical Review Fluids 7: 064202, 2022.

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Poster / 882

Effect of CO2 injection on porosity and texture of reservoir chalk assessed by 1H low-field gradient NMR measurements

Authors: Leonardo Teixeira Pinto Meireles[1]; Tobias Orlander[1]; Hanne Dahl Holmslykke[2]; Frederik Peter Ditlevsen[3]

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Chalk reservoirs are ubiquitous in the Danish north sea basin, making up to about 90% of the country's historical hydrocarbon reserves. Oil and gas production from these fields peaked in 2005, and they are expected to be abandoned within the next 10 to 20 years. The existing knowledge of the basin accumulated during over 50 years of exploration and development allied with the existing infrastructure makes these fields good candidates for geological CO2 storage. Nevertheless, carbonate reservoirs have been viewed unfavorably compared to clastic reservoirs regarding CO2 storage. This is because calcite is chemically unstable when exposed to weak acids, such as brine containing dissolved CO2, a likely scenario close to the CO2 saturation front.
In this study, we assess the permeability, porosity, and matrix texture changes along a chalk core subjected to seven alternating water and gas injection cycles (WAG cycles), using calcite-equilibrated formation water for the water phase and supercritical CO2 for the gas phase. Bulk Nuclear Magnetic Resonance (NMR) experiments were carried out before and after flooding, using a Geospec 2-53 NMR Core Analyser at the frequency of 2.25 MHz. The core analyser was equipped with a y-axis gradient coil, which allows the application of a varying external field to the core along its length, adding spatial resolution to the acquisition. This gradient coil was used to perform volume profile measurements and slice-selective T2 relaxation acquisitions.
Bulk NMR T2 relaxation distributions show an increase in total porosity, in agreement with porosity measured by helium expansion. The T2 relaxation distribution after flooding also indicates an increase in the sample's surface-to-volume (S/V) ratio, suggesting possible precipitation of fines and a decrease in sample permeability (Figure 1.A). This agreed with Klinkenberg permeability measured before/after the core flooding. Both NMR gradient-based measurements (Slice-selective T2 relaxation, not shown, and volume profile measurements, Figure 1.B) indicate that the gain in porosity is located close to the injection inlet. Towards the outlet, porosity is slightly lower than in the original core. Overall, the results show that gradient 1H low-field NMR measurements provide useful quantitative insights into textural changes happening within core plugs undergoing CO2 flooding.

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MS03 / 884

Condensation of vapor in a cracked sandstone revealed by in-situ rapid neutron tomography

Author: Arash NEMATI[1]

Co-authors: Bratislav Lukić [2]; Alessandro Tengattini ; Ritesh GUPTA [3]; Matthieu Briffaut [4]; Philippe Séchet [5]

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Among the processes that involve two-phase flow in porous media, phase change is less explored because of its complex nature due to the strong coupling between heat and mass transfer. Nevertheless, condensation processes are present in many fields, such as applications related to nuclear safety and durability of concrete structures, condensation in porous fabrics and insulations, steam-based gas recovery methods, underground contamination removal, and integrity of geothermal and CO<sub>2 storage reservoirs. Building upon the previous works on vapor condensation using high-speed neutron radiography (Lukic et al., 2021 and Gupta et al., 2022), in this work, 3D rapid *in-situ* neutron imaging acquired at 30 seconds per tomography is utilized to study condensation in a fractured sandstone. A predefined mixture of air and water vapor is injected at a constant flow rate into a cylindrical sample of Fontainebleau sandstone with a splitting crack along its height. The injection experiments were performed at the Institute Laue Langevin Grenoble (ILL) using the imaging instrument NeXT (Neutron and X-ray Tomograph) (Tengattiniet al., 2020). Successive rapid neutron tomographies are taken during the injection of vapor (2300 s) to investigate the water evolution inside the sample, and two higher resolution neutron tomographies are captured before and after the injection period to evaluate the overall condensed water. Furthermore, X-ray tomography is performed prior to the vapor injection, and part of the sample is scanned by synchrotron microtomography with a pixel size of 6.5 micrometers. This makes it possible to extract the microstructure and morphology of the crack and the porous matrix and evaluate the spatio-temporal accumulation of liquid water and its migration from the aspects of the crack and the matrix. The injected hot vapor cools down along its pathway toward the inlet of the sample causing the influx temperature to increase constantly. The condensation of the vapor fills up the pore space of the sample, thus a higher pressure is required to continue the vapor injecting as time passes. Water first appears near the inlet and propagates toward the further areas of the sample. The crack stays dryer compared with the areas around it, and the liquid water solely accumulates in the tighter areas with smaller widths inside the crack. The condensed water that is forming in and near the crack constantly diffuses into the porous matrix due to the capillary effect and the pressure buildup in the crack. Consequently, the areas near the crack accumulate more water content from the crack than the inner areas because the water content there exceeds the critical value and can be pushed away by the elevated pressure in the crack. The water front is measured and observed to linearly propagate both parallel and normal to the crack surface. Finally, the first results from a numerical model will also be introduced that further sheds light on the condensation process.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS23 / 885

Is salt precipitation an issue during geological storage of hydrogen in saline aquifers? from thermodynamic perspective using PC-SAFT EoS

Authors: Mohammad Masoudi[1]; Elyes Ahmed[2]; Xavier Raynaud[3]; Helge Hellevang[4]

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During the Underground Hydrogen Storage (UHS) process, hydrogen gas must be transported from the production site to the storage site, be injected into the storage repository (depleted hydrocarbon reservoir, aquifer, or salt cavern), and finally the stored hydrogen needs to be released from the storage site and be transported to the distribution points. During this long journey, hydrogen molecules can encounter a wide range of pressure and temperature and most likely be exposed to other fluids such as reservoir fluids, impurities, cushion gas, etc. In order to plan and perform risk analysis of UHS projects, it is necessary to model the phase behavior of hydrogen mixtures and accurately determine the distribution of hydrogen among different phases. Hydrogen gas (H2) has an ideal symmetrical structure and the phase behavior of pure H2 gas can be usually handled with Henry's law. Although, when H2 is injected to a depleted hydrocarbon reservoir or a saline aquifer or it is imposed to impurities during transportation, a more complex approach might be required to model the phase behavior of the mixture due to highly non-ideal intermolecular interactions, such as association (hydrogen bonding), polarity, ionic bonds, and chain forming reactions. In this work, we used PC-SAFT equation of state for this aim and added association, electrolyte, and polar contributions to the Helmholtz energy. We benchmarked the model against experimental data. A major advantage of the model is that it can be used for a wide range of pressures and temperatures, can handle non-ideal molecular interactions, especially when impurities are involved, and can apply to the entire chain of UHS.
Additionally, we have done a primary assessment of mutual solubility of H2 and brine to examine the possibility of dry out effect and salt formation during UHS in saline aquifers. The results show that the risk of salt precipitation is very low compared to CO2 storage in saline aquifers.

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In-Person

References:

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Poster / 886

Water imbibition in nanoporous Vycor glass: X-ray tomography-based Lattice-Boltzmann simulations and their validation by optical and gravimetric experiments.

Author: Juan Sanchez[1]

Co-authors: Mariia Liseanskaia [2]; Sahar Bakhshian [3]; Juliana Martins de Souza e silva [4]; Laura Gallardo [1]; Yannick Tetzner [5]; Andriy V. Kityk [6]; Martin Steinhart [7]; Dirk Enke [8]; Nima Shokri [9]; Patrick Huber [1]

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[5] *Hamburh University of Technology (TUHH)*

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Capillary rise dynamics of molecular liquids in nanoporous solid is governed by the interplay of liquid's viscosity, the liquid-solid interaction and permeability of the porous medium. Classical hydrodynamics provides a square-root-of-time dependent law to describe the liquid front advancement during imbibition, also known as Lucas-Washburn law (L-W). Although the validity of the L-W law down to the single digit nm scale has been proven 1, complex dynamics and broadening of the imbibition front arise in connection to the pore size distribution of the solid and its tortuosity.

To address this problem we present Lattice-Boltzmann computer simulations (L-B) of water imbibition in nanoporous Vycor glass. X-ray-based tomography of a 400 nm porous Vycor reveals the geometry of the pore space from the single-pore up to the Darcy scale. The scale invariant spinodal demixing-based pore formation in controlled pore glass allows us to re-scale such geometry $\sim$ 100 times down. Thus we complement the L-B simulations with optical imaging experiment for water imbibition in Vycor with poresizes of $\sim$ 4 nm. At this scale, changes in the refractive index of the solid upon filling provide for direct observation of the rise dynamics and the broadening of the filling front. The latter is visible via intense light scattering at this region induced by the coexistence of liquid-gas phases at length scales comparable to the light characteristic wavelengths.

Participation:

In-Person

References:

1 Simon Gruener, Tommy Hofmann, Dirk Wallacher, Andriy V. Kityk, and Patrick Huber (2009). Phys. Rev. E, 79(6).

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Energy Transition Focused Abstracts:

MS01 / 887

In Situ Imaging of Dynamic Processes in Chalk

Authors: Peter Winkel Rasmussen[1]; Benaiah Anabaraonye[2]

Co-authors: Nico Bovet [2]; Anders Nymark Christensen [1]

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Carbon storage (CS) in geological formations is a promising technology for mitigating climate change (IPCC, 2021). Historically, sandstone have been targeted for CS, but in the specific case of Denmark, chalk represents a more promising storage medium as it has a much higher storage potential (Bonto et al., 2021). Chalk, however, has a much higher reactivity with CO_2-saturated brines than sandstone. The interaction between the CO_2-saturated brine and the chalk can result in the dissolution and subsequent weakening of the chalk. This weakening can cause subsidence, which is detrimental to CO_2 storage (Liteanu et al., 2013). It is, therefore, imperative that the properties of chalk is studied in detail to verify its suitability for CS.

We designed a novel triaxial flow cell (shown in fig. 1) to enable in situ imaging of chalk. The cell is capable of maintaining up to 300 bar of pressure at 90 °C, which allows for the simulation of specific reservoir conditions. The central part of the cell is made of aluminium to maintain X-ray transparency. This is strictly necessary as it reduces the exposure time needed, which improves temporal resolution.
The temporal resolution of the CT scans is further improved by using the reconstruction algorithm presented by Rasmussen et al. (2021). This algorithm makes it possible to reduce exposure time and the number of projections without sacrificing image quality by utilising a high-quality reconstruction of the chalk sample. The high-quality reconstruction constrains the reconstruction of the in situ data, which improves image quality. Using this algorithm provides us with a temporal resolution of approximately 15 to 20 minutes.

The cell has been used for a series of non-reactive and reactive core flooding studies on reservoir chalk cores. Figure 2 shows the transport of a radiotracer (Cs_2CO_3) in a chalk sample. In the figure, we see two reconstructions of the chalk sample at different points in time. Note the bright band to the right in both figures is due to density variation in the chalk and is not caused by the radiotracer, unlike the bright region to the left in the images, which clearly advances during the experiment.

In fig. 3, we see the results from a triaxial compaction study. In this study, we slowly increased the triaxial pressure on a chalk core until it fractured, which occurred at approximately 82 bar based on the pressure drop recorded in fig. 3a. The fracture can easily be seen in fig. 3b, which shows a reconstruction of the sample after compaction. This study is valuable as it provides us with a baseline on which chalk weakened by CO_2 injection can be compared.

We demonstrate that our setup, in conjunction with the previously mentioned reconstruction algorithm, provide valuable insights into the suitability of chalk as a medium to store CO_2.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

890

Rarefied gas flow through the thin porous dust layer on the surface of comets

Authors: Omar Mokhtari[1]; Nicolas Thomas[1]

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Numerous studies and observations suggest the presence of a thin and highly porous layer of dust on the surface of comets that plays an important role in the outgassing properties and behaviour of comets. Located above the water ice sublimation front, this dust layer helps to explain a lower production rate and higher gas temperature at the comet surface (Christou et al. 2018). Unfortunately, very little is known about the constitution of the comet's surface, and the precise role of this porous structure remains difficult to understand. The idea is therefore to numerically simulate the flow of water vapour through different model porous media in order to understand which properties of the porous structure are most relevant. Ideally, we would like to be able to derive physical constraints on the properties of the dust layer on the surface of comets such as the thickness, particles size distribution and geometrical structure. As we are in a vacuum, the gas is in a rarefied form, i.e. the interactions between the gas molecules themselves are less frequent than those with the solid wall. The Navier-Stokes equations are no longer able to describe the flow. We therefore use the direct simulation Monte Carlo (DSMC) method to numerically simulate the flow through 2D cylinder arrays. After a study of role of the model parameters such as those describing the gas/gas and

gas/solid interactions, we focus on the role of the porous structure. Considering a large number of configurations we show that, independently of the rest, the two most important parameters are the thickness and the mean pore size thus confirming the validity of the Clausing's formula (Skorov et al. 1998 & 2011) initially established for capillary tubes. The disadvantage of this analytical formula is that it requires knowledge of the pressure and temperature at the surface of the comet, which are unknowns in the problem.
Beyond this validation, we highlight a coupling between the porous medium and the production rate which allows us to better understand the outgassing properties.

Participation:

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References:

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Energy Transition Focused Abstracts:

Poster / 891

Structural and transport properties of hydrocarbons in clay nanopores

Author: Vasily Pisarev[1]

Co-authors: Andrey Kalinichev [2]; Mikhail Logunov [3]

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[2] *Institut Mines-Telecom Atlantique, Nantes, France*

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Structure and transport of n-pentane and n-dodecane in clay nanopores are investigated using molecular dynamics (MD) method. OPLS-AA/CM1A force field 1 is used for hydrocarbons and ClayFF force field [2] is used to simulate pyrophyllite and montmorillonite pore walls.
The viscosity of hydrocarbons and slip lengths against the pore walls are calculated using non-equilibrium MD simulations of Couette flow. It is shown that the shear viscosity of n-pentane is only weakly affected by the pore walls for pore widths from 2 to 7 nm. The viscosity of n-dodecane increases in the pores.
The slip length of n-pentane against non-hydrated pyrophyllite walls is estimated at ~3 nm, while almost no slip is observed for n-pentane and n-dodecane against hydrated montmorillonite walls [3].
The orientational ordering of hydrocarons in pores is studied. Pentane molecules show weak ordering parallel to the walls in pyrophyllite pores and almost no ordering in montmorillonite pores with hydrated walls. On the other hand, dodecane shows strong ordering in pyrophyllite pores with molecules aligning in the same direction. The model shows a transition of n-dodecane into a state resembling liquid crystal at densities above 0.8 g/cc at 298 K [4].

The work has been supported by the Basic Research Program of the National Research University Higher School of Economics.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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Experimental investigation of the impacts of net stress on pore confinement effects on the effective dew point pressure of gas condensate mixtures

Authors: Hosein Doryani[1]; Mahmoud Jamiolahmady[2]

[1] *Institute of Petroleum Engineering, Heriot Watt University*

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With increased energy demands for future, the importance of the role of unconventional gas resources cannot be overstated. Recent technological advances, including horizontal well drilling and hydraulic fracturing, have facilitated hydrocarbon recovery from unconventional reservoirs. However, it is necessary to study the phase behaviour and flow of fluids within these reservoirs, as they are not well understood. More specifically, much higher reliable experimental data are needed to confirm/modify the existing theoretical models.

The average pore size of conventional porous media is in the range of micrometre, which is several orders of magnitude higher than the fluid molecule diameters. As a result, in conventional reservoirs, the extent of the interactions among fluid and pore walls molecules, may be neglected compared to that taking place between fluid molecules. In tight and shale reservoirs, on the other hand, the pore sizes are comparable with the sizes of the fluid molecules. Therefore, the frequency collision between fluid and pore walls molecules are more and their interaction cannot be ignored. Fluid confinement is the term used to describe interactions for a system of fluid molecules whose phase and flow behaviours are affected by the surfaces of the void space of the pores and fluid phase properties cannot be captured by conventional methods used for conventional reservoirs.

We have recently designed and proposed a novel experimental method to measure the effective dew point pressure (Pdew) of hydrocarbons inside real porous media [Jamiolahmady, M. et al. (2020), Jamiolahmady, M. and Doryani, H. (2021)]. In this experimental research, the impact of net stress on the extent of fluid confinement on the phase behaviour of a gas condensate sample within a real shale core sample was evaluated. Bulk Pdew of the binary gas-condensate fluid sample was measured to be 4052 psi with MLDO of 24 %. The core flood experiments were designed and carried out at three

different net stress values of 500, 1000, and 2000 psi. It was observed that due to increased net stress, the difference between bulk Pdew and effective Pdew increased from at least 129 psi for net stress value of 500 psi to 147 psi for net stress values of 1000 psi and 2000 psi. These results revealed that increasing net stress increased the extent of the effects of pore confinement on increasing trend of effective dew point pressure inside porous media.
The results of this novel experimental study sheds light on the extent of pore confinement effects. This study, for the first time, experimentally demonstrates that in real unconventional shale samples, geomechanical effects not only have significant effects on the fluid flow in porous media but also they impact the phase behaviour of hydrocarbons inside the nano- and micro-pores of porous media.

Participation:

Online

References:

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893

Evolution of water films on mineral surfaces in partially-saturated porous media

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Water films on mineral surfaces affect physical, chemical, and biological transport processes in atmosphere, soils, and rocks. The aim of this study, regarding unsaturated flow and transport in geological media, is to understand how the adsorbed water phase evolves as a function of relative humidity, mineralogy, ionic strength, and temperature. Experimentally measured water film thicknesses in the literature range from several angstroms to few hundred nanometers depending on relative humidity, solution chemistry, and electrostatic potential of mineral surface. The equilibrium film thickness appears to be highly sensitive to vapor pressure values near the saturation value and increases exponentially as the relative humidity approaches unity. However, the data typically are limited to film thicknesses measured on single mineral crystals at low temperatures (< 25 ^{o}C). The magnitudes of intermolecular forces between water molecules and the van der Waals and electrostatic interactions between water and mineral surfaces control the evolution of adsorbed water phase and water film thickness under different temperatures. Unlike existing models for predicting equilibrium water film

thickness based on the Derjaguin–Landau–Verwey–Overbeek (DLVO) theory, this study presents a dynamic model based on the square-gradient classical density functional theory. The model, which consists of coupled partial differential equations for transport of water, chemical potential and the Poisson-Boltzmann equation, can be used to understand and predict evolution of water films on mineral surfaces and in porous media. The presentation of this study will include numerical applications of the model to interpret experimental data of water film thicknesses and give insights on evolution of adsorbed water phase under different environmental conditions.

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Energy Transition Focused Abstracts:

MS03 / **894**

Bridging the gap between lab experiments and mixed-dimensional modeling for flow and transport in fractured media

Authors: Jakub Both[1]; Bergit Brattekås[2]; Martin Ferno[1]; Eirik Keilegavlen[1]; Jan Martin Nordbotten[1]

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The existence of fractures in porous media has a strong impact on the characteristics of the flow behavior. In geological rocks, fractures occur both naturally as well as intentionally induced as in geothermal applications. Thus, accurate modeling and simulation of flow and transport in fractured media is vital for many industrial applications.

Mixed-dimensional models have been widely used for modeling flow in fractured media. The high aspect ratio of the fracture width as compared to their remaining dimensions allows for representing them as lower-dimensional manifolds. By combining the fundamental principle of mass conservation and Darcy's law on each subdomain and mass transfer inbetween domains, underlying equidimensional models can be conveniently replaced. Yet, despite the large interest in mixed-dimensional models for flow and transport in fractured media, direct comparisons to high-quality lab experiments have been missing.

In this talk, we present such a comparison study based on PET experiments of tracer transport in fractured sandstone and corresponding numerical simulations of mixed-dimensional flow and transport (PorePy). In addition, we present tailored image analysis (DarSIA) used to transfer PET images to Darcy-scale images and to compare different Darcy scale images by suitable metrics.

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Energy Transition Focused Abstracts:

895

Prediction and Real-Time Optimization in Biogas Production Plants with Circulating Flow

Authors: Babett Lemke[1]; Arne Naegel[2]; Falko Niebling[3]; Michael Tietze[3]; Gabriel Wittum[4]; Rebecca Wittum[5]

[1] *TechSim UG*

[2] *Goethe-University Frankfurt*

[3] *GICON Großmann Ingenieur Consult GmbH*

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Background/motivation: The complex biology of processes in biogas production plants (BPP) has been an active field of research for many years. Often an increase of both process efficiency and operational stability are primary concerns. Here modelling and simulation are attractive techniques, that can contribute in various settings. This includes, e.g, optimising feeding schedules for flexible production in existing plants, or assessing design decisions when plants are extended. Moreover, modelling provides am means for operational stability and prognosis options in complex trading scenarios for renewable resources with sector coupling 1.

Aim of the work: Develop a modelling tool serving as a guidance to BPP design and operation. Estimate the current state of the BPP based on a small subset of parameters. Adjust parameters, if required. Facilitate predictions for plant design, construction and operation.

Key research topics and novelty: In this work, we present a framework for the simulation of a BPP arranged in a network of coupled reactors and storage devices. The close interaction with optimization tools allows for parameter identification and control. This allows to control the operation in a semi-automated fashion.

Methodology: We consider a genuine biogas production plant that is operated under circulating flow conditions. The plant consists of a network of coupled reactors that connected by active and/or passive elements, e.g., overflow tubes or programmable controls. Mathematically, this is modelled and expressed as a graph.

In contrast to classic ADM1-type models, cf. [3,4] for an overview, the model features full spatial resolution of the reactors'interior [2]. This provides information on the heterogeneous composition of the circulating fluid. Depending on the physical dimensions of the reactors and the prescribed flow rates, this is important, e.g., for investigations on the impact of feeding or for the evaluation of sensor placement.

The long term goal of this work is to facilitate simulations on state-of-the-art workstations. In order to meet real-life run time requirements, model reduction techniques are employed. At the user' s discretion, full resolution volume-type 3D reactors can be replaced by line-type 1D flow through reactors. In the simulation framework, both approaches coexist and are compared. This is important when evaluating different configurations, for instance plug-flow, batch or CSTR reactors.

For treating data uncertainty, an optimization component is an essential: First, all sub-units, must be calibrated beforehand. This can be achieved, e.g., based on existing data and batch experiments. Second, it may be required to adjust the model on the flight. To that end, we extract short time series, and adjust parameters on the flight.

Results: We provide results for a genuine plant. Model features of are demonstrated and numerical experiments and real-world BPP data are intertwined. Predictions and hypothesis testing both w.r.t. design and operation mode, as well as the semi-automated control flow is demonstrated. Strategies for an application of the model for existing plants and the economic impact are discussed.

Participation:

Online

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MS01 / 896

Pore-scale observations of hydrogen trapping and migration in porous rock

Author: Yihuai Zhang[1]

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We use high-resolution three-dimensional X-ray imaging to study hydrogen injection and withdrawal in the pore space of Bentheimer sandstone. The results are compared with a replicate experiment using nitrogen. We observe less trapping with hydrogen because the initial saturation after drainage is lower due to channelling. Remarkably we observe that after imbibition, if the sample is imaged again after 12 hours, there is a significant rearrangement of the trapped hydrogen. Many smaller ganglia disappear while the larger ganglia swell, with no detectable change in overall gas volume. For nitrogen, the fluid arrangement seems largely unchanged. We suggest that this rearrangement is facilitated by concentration gradients in the aqueous phase –Ostwald ripening – and provide an estimate of the time-scales for the effect to be significant, which are consistent with the experimental observations. The work implies that there is less capillary pressure hysteresis in hydrogen storage, promoting hydrogen withdrawal efficiency.

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Poster / 897

Molecular Mechanisms Underlying The Treatment of Archaeological Wood Cell Wall Composite with Polyethylene Glycol: A Hybrid Monte Carlo and Molecular Dynamics Study

Author: Ali Shomali[1]

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Treatment of wood cell wall with polyethylene glycol (PEG) is a widely used technique by archaeologists and conservators to consolidate waterlogged archaeological wooden artifacts such as the Swedish warship Vasa and Henry VIII's warship the Mary Rose. During the decade-long consolidation process of introducing PEG solution into these wooden artifacts, PEG molecules gradually diffuse into the wood cell wall and replace the water molecules. PEG treatment is found to stabilize the wood structure and prevent extreme shrinkage and structural collapse during the following slow drying process altering the hygromechanical properties of wood in response. Due to the chemical complexity and hierarchical intricacy of the wood structure, PEG-cell wall interactions are governed by various entangled multi-scale mechanisms which are yet to be elucidated and distinguished.
This work attempts to provide a molecular-level understanding of the impact of PEG treatment on the hygromechanical properties of wood-cell wall components, including amorphous cellulose, hemicellulose (galactoglucomannan), uncondensed lignin (coniferyl and sinapyl) and fiber-matrix interphase. To this aim, an iterative hybrid all-atom molecular dynamics and grand canonical Monte-Carlo (GCMC) simulation is employed to examine the hygromechanical properties of polymeric mixtures, including sorption isotherm and sorption hysteresis and sorption-induced swelling. The structure of mixtures of biopolymers and PEG equilibrated under a range of relative humidity from fully dry to saturation is then characterized by measuring porosity, pore size distribution, mechanical properties, and hydrogen bonding network.
The amorphous cellulose mixtures treated with PEG show reduced moisture adsorption and swelling at museological conditions (40-60% RH), followed by an unfavorable increased sorption/swelling at high relative humidity, highlighting a crossover phenomenon in hygroscopicity. In comparison, lignin mixtures show less substantial moisture/swelling reduction indicating that PEG treatment is more effective on polysaccharide polymers of wood. The cellulose nanocomposite model reveals the concentration of PEG at the fiber-matrix interface, which disturbs the fiber-matrix hydrogen bonding network and consequently enhances the moisture sorption and mechanical softening at the interface. Comparing the simulation results with predictions from an enhanced rule of the mixture model reveals the key role of interphase and synergic interaction between PEG and wood polymers. The enhanced mixture model enables us to characterize two molecular mechanisms governing the consolidation at the nanoscale. First, the filling of existing nano-sized pores in the amorphous structure by PEG as relatively small PEG molecules fill the vacancies previously available for the adsorption of water molecules. Second, the network of wood polymers confines PEG polymers and prohibits PEG from further swelling, thus reducing its water sorption. This behaviour of PEG may be a characteristic to look for when considering novel consolidant materials in the future.

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MS15 / **898**

3D Reconstruction of Porous materials using Deep Learning

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Precise 3D demonstration of heterogeneous porous materials while critical is still a challenge. The advantage of having such models includes for example more accurate characterization and estimation of transport properties. Realistic 3D representations can be achieved using several high-resolution 2D samples. We applied a deep learning algorithm to utilize 2D images and reconstruct 3D models of complex materials such as lithium-ion battery electrodes. The deep learning algorithm was trained using 2D images for generating 3D samples. The results of testing the trained network with new samples show the capability of the algorithm for reproducing important structural properties. The reconstructed samples also reproduce the results for flow and heat properties in an acceptable range.

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MS07 / 899

A linear iterative scheme for reactive flow in a porous medium

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We consider a mathematical model for saturated flow and reactive transport in a porous medium. In this model, the absolute permeability of the medium depends on the solute concentration. Due to this, the fluid velocity depends on the unknown concentration. On the other hand, the solute is transported by the fluid, so the concentration is dependent on the fluid velocity. This yields a fully coupled system of nonlinear partial differential equations.

After appying an implicit Euler time stepping, one obtains a sequence of nonlinear, fully coupled time-discrete systems of elliptic equations. We propose a robust, linear iterative scheme for the numerical approximation of the solution to the time discrete systems. By adding some linear stabilization terms, one not only makes the scheme linear, but the two components of the model, the flow and the reactive transport of the solute, can be decoupled. Under a mild restriction on the time step, we prove the convergence of the iterative scheme. This convergence holds regardless of the spatial discretization and mesh.

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Energy Transition Focused Abstracts:

Poster / 900

Pore-scale imaging of nonlinear multiphase flow in porous media

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Multiphase flow in porous materials is conventionally described by an empirical extension to Darcy's law, which assumes that the pressure gradient is proportional to the flow rate. Through a series of bench and pore-scale imaging two-phase flow experiments, we demonstrate that even when capillary forces are dominant at the pore scale, there is a nonlinear intermittent flow regime with a power-law dependence between pressure gradient and flow rate. Energy balance is used to predict accurately the start of the intermittent for a range of fractional flows, fluid viscosities, and different rock types. The pore-scale explanation of the behaviour based on the periodic filling of critical flow pathways is also confirmed through 3D micron-resolution X-ray imaging.

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MS06-A / 901

Characteristics of fluid-fluid displacement in model mixed-wet porous media

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Fluid-fluid displacement in porous media occurs in many natural and engineering processes such as geological CO2 storage and enhanced oil recovery. It has been recognized that wettability plays an important role in the displacement process. Thanks to decades of research, we now have a good understanding of fluid-fluid displacement in porous media with uniform wettability. In contrast, our knowledge of fluid-fluid displacement in porous media with heterogeneous wettability (i.e., mixed-wet) is much less complete, even though mixed-wet conditions are common in many subsurface processes.

Here, we study fluid-fluid displacement in simple mixed-wet micromodels. The micromodels are made of an oil-wet polymer whose wettability can be locally tuned to become water-wet via deep UV exposure. Our experiments show the mixed-wet pores exert fundamental control over the macroscopic displacement pattern and that the incorporation of the capillary entry pressures at mixed-wet pores into a dynamic pore-network model reproduces the experiments. Using the pore-network model, we systematically vary the fraction of water-wet to oil-wet regions and obtain a variety of displacement patterns over a wide range of Ca. We find that the impact of mixed-wettability is most prominent at low Ca, and it depends on the complex interplay between wettability fraction and the intrinsic contact angle of the water-wet regions. Mixed-wettability is also manifested in the injection pressure signature, which exhibits fluctuations at low wettability fractions. Finally, we demonstrate that scaling analyses based on a weighted average description of the overall wetting state of the mixed-wet system can effectively capture the variations in observed displacement pattern morphology.

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In-Person

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Energy Transition Focused Abstracts:

902

Thermo-mechanical model of second-graded porous materials: A higher-order homogenization approach

Author: Bozo Vazic[1]

Co-author: Pania Newell [1]

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Many novel engineering materials such as metal foams, glass ceramics, or hemp fiber-reinforced concrete are classified as porous materials and are widely used in many areas of applied sciences and engineering. Porous materials with diverse structures possess a wide range of mechanical, thermal, or electrical properties. Therefore, they have been utilized in many engineering fields, from energy-storage technologies and geothermal engineering to bio-engineering. The development of reliable multi-physics models for porous materials requires understanding the fundamental mechanisms and proper application of modeling techniques. Due to the strong influence of pore morphology on material properties, over the years, a wide range of analytical and numerical homogenization techniques have been developed to efficiently upscale material properties from micro- to macro-scale. Most of these homogenization techniques are based on averaging a physical field, such as stress, strain, and deformation energy density. However, since they are mostly based on the classical continuum theory, their capabilities are limited as they are only able to capture the absolute size and distribution of the pores. In this work, we adopt a higher-order asymptotic homogenization method that is an extension of the first-order computational homogenization framework based on a generalized continuum. By introducing a length scale into the material constitutive law, the higher-order approach allows us to capture the absolute size of pores and pore distribution when upscaling both displacement and temperature fields. Similar to our previous research on the influence of micro-pore morphology on mechanical properties, Vazic et al. [2022], we have employed a thermo-mechanical model on a set of numerical problems with different combinations of porosity, pore shapes (i.e., circular and elliptical), and with different distributions (i.e., single pore and uniform/random distribution). These cases showed that thermoelastic interaction, β^M, has a similar sensitivity to pore morphology as the stiffness matrix, C^M, while higher-order thermal parameters, γ^M, mirror the response of the higher-order mechanical parameter, G^M, as both of them are linearly dependent on the size of the RVE and have the same behavior with respect to the centro-symmetry of the RVE. This theoretical framework and its numerical implementation will serve as a platform for future research to better understand the interplay between microscale morphology and thermo-mechanical material parameters.

Participation:

Online

References:

Vazic, B., Abali, B.E. and Newell, P., 2022. Generalized thermo-mechanical framework for heterogeneous materials through asymptotic homogenization. Continuum Mechanics and Thermodynamics, pp.1-23.

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Poster / 903

Non-Newtonian fluids based method for characterizing the pore structure of spherical glass bead particles

Authors: Soheil Safari Anarkouli[1]; Martin Lanzendörfer[1]; Martin Slavík[2]; Tomáš Weiss[2]

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Transport processes and mechanical properties of porous media are extensively related to microscopic features of the pore structure, and especially to the pore size distribution (PSD). Unlike with other soil characteristics, e.g., porosity and specific surface area, for which there is a consensus over the estimation approach, the available methods for estimating PSDs are often costly and instrumentally demanding while having specific limitations in terms of applicability or, e.g. the laboratory sample preparation 1.
With micro-computed tomography (μCT) limitations in terms of spatial resolution and cost, toxic mercury intrusion porosimetry is nowadays the prevailing technique to determine PSDs of most porous media. Recently, using non-Newtonian fluids for obtaining the PSD of porous media has been identified as a promising safe, and cheap alternative method to MIP and micro-CT. Despite water (as a Newtonian fluid), the flow of some non-Newtonian fluids through porous media is related to the geometry of the pores in a way that allows backtracking of some information, particularly the approximate distribution of the effective pore sizes. This can be (and has been) done in various ways, cf. The yield stress fluid porosimetry method (YSM) [2], extracts the PSD of a given material from the pressure drop vs. flow rate measurements during injection of a yield stress fluid, or more recently the model presented by Abou Najm and Atallah (ANA model) [3], derives the effective pore size distributions of the porous sample based on a set of saturated flow experiments with different shear-thinning fluids.
This project will be based on both laboratory experiments and computational modeling, with an emphasis on the link between the experiments and the modeling.
In the experimental part, we will apply the ANA method to synthetic porous media systems to assess the model's ability to characterize the pore structure, both in terms of producing accurate pore radii and in providing more information than would be available from traditional, single-fluid based approaches [4]. A series of one-dimensional column experiments will be conducted with varying porous medium packings consisting of spherical glass bead particles in mono-sized and binary mixtures. For each packing, distilled water and varying concentrations of xanthan gum will be injected over a range of flow rates and pressure gradients.
In the numerical part, the discrete element method (DEM) will be used to generate random packings of mono-sizes and binary mixtures of spheres in cylindrical columns. Subsequently, having the simulated configuration of grains in each packing, the pore network (pore body and pore throat) will be extracted using different image analysis algorithms, and computational fluid dynamics (CFD) approaches [5].
We are particularly interested in how the extracted pore networks from some available image processing techniques will be represented by the effective PSD obtained by the ANA method to compare their performance on a selection of synthetic images of packs of spherical glass beads.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

904

A Neural Network Model to Predict Nonlinear Dynamics and Deterministic-Chaotic Gas Migration in Bentonite

Author: Boris Faybishenko[1]

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We analyzed the results of the gas injection experiment in the Mx80 bentonite core, which was conducted at the British Geological Survey, and calculated a set of the diagnostic parameters of nonlinear dynamics and chaos of univariate temporal trends of gas pressure and gas influx (i.e., input to the core) and outflux (i.e., output of the core). Because it is not possible to derive analytical forecasting models for processes exhibiting chaotic behavior, we performed simulations and forecasting of time series based on using lagged input time series to fit neural network models to time series of observed temporal trends. The optimal time-lag (i.e., time delay) of each analyzed time series was determined using the average mutual information (AMI) method. Then, we created three-dimensional (3-D) datasets consisting of a recorded time series, time series with time minus one time lag, and time series minus two time-lags. These datasets correspond to the 3-D pseudo-phase attractors, approximating the time-delay dynamics of the system. We tested the application of single layer and two-layer neural network models trained using several methods – backpropagation, resilient backpropagation with or without weight backtracking or the modified globally convergent version. The forecasting accuracy was determined using several statistical goodness-of-fit measures, such as the RMSE, MAE, MAPE, SMAPE. A baseline for the evaluation of the accuracy of forecasting was based on the application of the generalized linear regression model. 2-D and 3-D pseudo-phase space attractors for observed and predicted time series are used to demonstrate graphically the accuracy of predictions. Thus, we show that a neural network approach can be used for long-term predictions of nonlinear dynamics and deterministic-chaotic time series of gas flux through bentonite.

Participation:

Online

References:

Faybishenko, B., Wang, Y., Harrington, J. et al. Phenomenological Model of Nonlinear Dynamics and Deterministic Chaotic Gas Migration in Bentonite: Experimental Evidence and Diagnostic Parameters. Transport in Porous Media, 141, 585–606 (2022). https://doi.org/10.1007/s11242-021-01733-9

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Energy Transition Focused Abstracts:

Poster / 906

Reservoir-scale simulation of CO2 solutal convection: approaches and limitations

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The CO2 dissolution in the reservoir brine (eg. within an aquifer) is one of the primary trapping mechanisms during CO2 geological storage (CGS). Significant amounts of injected CO2 can be trapped in this way with the overall dissolution rate controlled by density-driven convective mixing (CM). As such, the CO2 solutal convection results from the gravitational instability: under the action of buoyancy the injected CO2 displaces reservoir brine from the reservoir top so that denser CO2-saturated brine is found above a less dense original brine [1,2]. As a result, the typical dynamic CM pattern includes descending fingers of CO2-saturated brine surrounded by ascending volumes of original reservoir brine and accompanied by the progressive CM of CO2 [3].
After nearly 30 years of compehensive research efforts where significant part of results on the CO2 convective mixing was obtained via numerical analysis (cf. [4]), the reservoir-scale simulation remains surprisingly scarce while dedicated reservoir simulators are generally poor in adequate description of more or less realistic CGS scenarios comprising the long-term dynamics of CO2 dissolution [5].
The main objectives of our current work were (1) to summarize the successful approaches to realistic large-scale modelling of the CM during CGS (cf. [6]); (2) to understand the origin of principal restrictions which make inefficient the dedicated simulators, and (3) to specify possible ways to enhance existing simulation models in order to estimate, for instance, the impact of CO2 dissolution on the dynamics of the plume size and/or the CO2 storage. The essential result of the steps (1) and (2) was the development of 3D computationally efficient model of the CM; in particular, besides the study of dynamic dissolution regimes occurring after the solutal convection onset (eg. under the typical Utsira conditions), the model has been applied for the realistic size and physical properties distribution cases, cf. [7]. The direct comparison to dedicated simulators has demonstrated the limits in their accuracy and computational performance. At the same time, it was found that a study of such a kind may indicate the direction of possible model improvements. The necessary methodological elements to be taken into account or to be developed and incorporated to the general workflow are discussed in some detail together with examples demonstrating their application.

Participation:

In-Person

References:

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MS02 / **907**

The role of root hairs in root water uptake - Insights from an image-based 3D model

Author: Patrick Duddek[1]

Co-authors: Mutez A. Ahmed [2]; Mathieu Javaux [3]; Jan Vanderborght ; Andrea Carminati [1]

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[2] *UC Davis, Department of Land, Air and Water Resources*

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Plants acquisition of soil resources such as nutrients and water will be severely impeded in the near future as a consequence of climate change. Root hairs, tubular extensions of epidermal root cells, substantially increase the contact area between roots and soil and are hence considered a key rhizosphere trait increasing the capacity of plants to capture soil resources. While their pivotal role in the uptake of immobile nutrients such as phosphorus is well accepted, their effect on root water uptake remains controversial as it varies across plant species.

By means of image-based modelling, our objective was to identify environmental conditions (e.g. soil water content) and hair traits (e.g. root hair length and density) that determine the effectiveness of root hairs in root water uptake. Furthermore, we investigated the effect of drought stress-induced root hair shrinkage on root water uptake.

Using synchrotron radiation X-ray CT, we scanned root compartments of 8 days old maize seedlings (*Zea Mays* L.) grown in loamy soil, a complex porous medium. The acquired image-data served as a basis for our image-based 3D root water uptake model. By solving Richards equation numerically, we computed the propagation of water potential gradients across the root-soil continuum. The high spatial resolution of the acquired images allowed to explicitly take rhizosphere features, such as root hairs, root-soil matrix contact and aggregate structure into account. To determine the key parameters governing the effectiveness of root hairs in water uptake, we compared a set of six maize root compartments of approx. 1.4mm length before and after digitally removing their hairs. The quantification of root hair turgor-loss in response to progressive soil drying allowed us to implement hair shrinkage within our model.

We found that the effectiveness of root hairs in root water uptake mainly depends on 1) the root hair induced increase in root soil contact and 2) root hair length. Furthermore, our results suggest that root hairs potentially facilitate root water uptake under dry soil conditions (< -0.1MPa). However, in

the dry range, root hair shrinkage severely impairs the effect of hairs. Depending on the turgor-loss curve, root hairs may still provide a positive effect on root water uptake in a narrow range of soil matric potential.

In summary, the effect of root hairs on root water uptake is determined by soil water content, root-soil contact, root hair length and the turgor-loss point of hairs.

Participation:

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Energy Transition Focused Abstracts:

Poster / 908

A Size-Structured Approach for Filtration Modelling

Author: Connor McAllister[1]

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Filtration is a well-researched industrial process in which solid particles are separated from a fluid by becoming trapped within the filter's internal structure. Recently, mathematical models have offered a cost-effective means to advance understanding of the filtration process and improve filtration performance. However, many models exhibit shortcomings which include large computational costs and an inability to incorporate multiple capture mechanisms. To negate these deficiencies, we explore a size-structured approach for modelling particle filtration in which size is treated as an independent variable .

In this paper, we outline the derivation of a size-structured model and analyze the system of equations for several filtration configurations. We demonstrate the distinct filtration behaviours induced by the various capture mechanisms and, for certain cases, exploit the size of material parameters by using asymptotic analysis to find analytic solutions. Furthermore, we illustrate the model's predictive potential to maximize particle retention given an efficiency constraint. Finally, we explore how the model's dimensionless parameters influence the degree to which it fits with experimental data.

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Energy Transition Focused Abstracts:

Poster / 909

Design of Colloidal Gas Aphron Drilling Fluid Formulations for Enhanced Deep Geothermal Energy Recovery Operations

Authors: Igor Paevskiy[1]; Ian Collins[1]; Edo Boek[2]

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Drilling operations required for recovery of deep geothermal energy are often challenging. This is due to the harsh downhole conditions encountered in geothermal wells, including high-pressure-and-high-temperature (HPHT) and the toughness of the rock found in many geothermal formations. Drilling in such environments requires special drilling fluid formulations that have high thermal stability, good rheological properties, and excellent lubricity. A review of the literature reveals two commonly observed problems in deep geothermal drilling operations, significantly increasing drilling costs: a) **lost circulation** of drilling fluids in highly permeable fractured rock formations and b) very **low Rate of Penetration (RoP)**. Our literature review shows that RoP can be significantly improved by underbalanced drilling using low viscosity and low-density drilling fluids, such as **foams** and **Colloidal Gas Aphron (CGA)** systems (Zhu et. al., 2019). Note that such systems to date have only been studied at relatively low temperatures and the challenge of increasing the thermal stability of the formulation components needs to be addressed. Here we investigate novel CGA systems and report preliminary results on the stability and rheological properties of novel CGA formulations. In particular, we investigate the effect of laponite as a thermally stable alternative to Xanthan Gum (XG) as a drilling fluid viscosifier. A domestic high shear homogeniser was utilised in this study, which to our knowledge is a novel approach following low-cost innovation principles. The advantages of this approach include higher degree of homogenisation and mixing speed tuneability compared to other household mixers commonly used in the literature. First, we observe that the resulting CGAs have low measured densities of 0.43-0.56 g/ml, allowing underbalanced drilling conditions. Second, all CGA drilling fluid formulations demonstrated shear thinning behaviour, following the Herschel-Bulkley rheological model. Third, our formulations after aphronisation showed demonstrably higher low shear rate viscosities (LSRV) than before, which is a desirable property for any drilling fluid. Fourth, we observed that laponite has a positive effect on the LSRV in drilling fluids, and also supports the formation of CGAs. Our study proved that laponite is an effective viscosifier in combination with organic polymers such as XG. Future research will investigate whether XG can be substituted with laponite, as this enhances the thermal stability of drilling fluids (Huang et al., 2019). Fifth, and most importantly, we observed that the surfactant chosen to stabilise the CGA suspensions influences the size distribution of aphron bubbles in solution. In all samples, the use of SDBS results in a larger bubble count compared to SDS. In addition, SDBS shows a narrower size distribution of bubbles, see Fig.1. To **minimise lost circulation of drilling fluids** in highly permeable fractured geothermal reservoir formations, a **larger bubble count** is a positive factor with respect to rock formation sealing capabilities of the drilling fluid. However, an optimal **CGA bubble size distribution** will depend on the **pore size distribution (PSD)** of the rock formation. Here we propose that CGAs can potentially be designed as Lost Circulation Materials (LCM), by **tuning bubble size distributions to match the PSD** in fractured geothermal reservoir formations.

Participation:

In-Person

References:

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MS05 / 910

Recent insights on the coupled processes and potential applications of microbially induced desaturation and precipitation by nitrate-reducing bacteria

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Microbially induced desaturation and precipitation (MIDP) is investigated for several engineering applications in porous media. The MIDP process involves injecting a nutrient solution containing calcium acetate and calcium nitrate in the subsurface, which stimulates indigenous nitrate-reducing bacteria to convert these substrates into three main products: biogenic gas (mainly nitrogen and some carbon dioxide), biomass and calcium carbonate biominerals. Each of these products affects the hydraulic and mechanical properties of porous media. Biogenic gas desaturates the soil, which increases the compressibility of the pore fluid, which dampens pore pressure build up during cyclic loading of loose granular soils and can therefor be used to mitigate earthquake-induced liquefaction. Precipitation of calcium carbonate minerals increases strength, stiffness and dilatancy precipitation of unconsolidated sediments; and all three phases, biogenic gas, biominerals and biomass fill up the pore space and reduce the hydraulic conductivity. This contribution highlights recent studies, which demonstrated how the distribution, migration and permanence of biogenically formed gas is affected by the reaction rate, the grain- or pore size distribution and pore connectivity and at a larger scale by overburden pressure and soil stratification. Lab tests demonstrated that only a 10% reduction in degree of saturation is sufficient to significantly increase the undrained cyclic shear resistance of loose sands, while field tests demonstrated that MIDP treated sediments remained desaturated for more than 3 years. A simplified numerical model was developed and used to simulate the biochemical conversion and predict its affect on the hydraulic and mechanical properties. The model was fitted on experimental data and simulations suggested that the coupled interaction between the different phases resulted in very efficient clogging showing a permeability reduction of two orders of magnitude with only 1 wt% of calcium carbonate. When multiple treatment cycles are applied or multiple pore volumes are injected, local changes in hydraulic conductivity affect the distribution of substrates and products, particularly during the first few cycles.

Participation:

In-Person

References:

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Poster / 913

Atomistic computer simulation of the structure and properties of iodine and chlorine containing hydrocalumite (AFm phase) as adsorbent for radionuclides 36Cl, 129I, 137Cs

Authors: Artem Glushak[1]; Grigory Smirnov[None]; Evgeny Tararushkin[1]; Andrey Kalinichev[2]

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AFm phases of hydrous Ca-aluminates Ca2Al(OH)6·Cl·2H2O (also known as hydrocalumite) and Ca2Al(OH)6·I·2H2O were considered as adsorbent for radioactive anions. The layered structure of hydocalumite is formed by distorted Ca-hydroxide and Al-hydroxide octahedra. Its interlayers are formed by a highly ordered arrangement of Cl- anions and H2O molecules. It is structurally one of the best understood of the layered double hydroxides (LDHs) and can serve as a good model for other less ordered natural and synthetic LDH phases important for a wide variety of technological applications, such as environmental remediation, while only experimental studies of iodine-containing AFm phases have been conducted.
In this work we studied hydrocalumite with chlorine and iodine anions in interlayer space as adsorbent for radionuclides 36Cl, 129I, 137Cs via molecular dynamics simulations. Performed computer simulations allowed us to study both crystals properties and interaction of the same crystals with

aqueous solutions of CsCl and CsI.
The structural and dynamic properties for both systems were modelled with the ClayFF-MOH force field model that is capable of realistically describe all interatomic interactions in such systems and which can now more accurately account for the bending of Al–O–H and Ca–O–H angles in the mineral structure. Our results are confirmed with earlier atomistic simulations of hydrocalumite which were among the first successful applications of the ClayFF force field model.
Study reported that stronger adsorption of Cl-, compared to adsorption of I-, leads to partial adsorption of Cs+ cation. This can be explained by the difference in van der Waals radius of Cl and I that make up 175 pm for Cl and 198 pm for I. In addition, the diffusion decreases by an order of magnitude at a distance of 3 A, which is consistent with previous works.

Participation:

In-Person

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916

Microstructural evaluation of digital geological materials using ImageJ software

Author: Raquel Benevides Dias Lima[1]

Co-authors: Elaine Cristina Gomes Barreto [2]; Janine Domingos Vieira [1]

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In the field of materials engineering, there is a growing interest in the development of computational methods for microstructural evaluation. The three-dimensional scanning of materials using

X-ray micro-computed tomography (micro-CT), in addition to being a non-destructive sample technique, presents a range of possibilities for analysis, allowing the measurement of textural parameters and physical properties. One textural analysis is the pore size distribution, as an alternative to performing a conventional laboratory test of mercury intrusion porosimetry (MIP). For this, the use of microCT image processing software is necessary. There are several commercially available software with this purpose. However, it can be highlighted the potential for using the open source program called ImageJ, developed in Java at the National Institutes of Health, in the United States, and constantly fed with the academic cooperation of several multidisciplinary researchers and users worldwide, developing plugins and macros for processing and extracting attributes from 2D and 3D images. In this context, this work proposes a method for microstructural evaluation of four geological materials –two rocks: sandstone and carbonate, and two soils: sand and clayey soil –digitized by micro-CT, in terms of porosity, size, and shape of pores, using the ImageJ program. Thus, the workflow includes: (i) pre-processing, in which images and desirable characteristics are enhanced; (ii) segmentation into phases of interest –in particular, porosity -, using a machine learning tool; (iii) post-processing, separating the objects of interest into individual three-dimensional elements; (iv) attribute extraction, in which size and shape measurements are made of these objects. From these measurements, the engineer performs statistical analyzes that allow a better interpretation of the measurements (volume, surface area, sphericity, elongation) and presentation of the textural parameters of the pore network (pore radius distribution and grain shape). The results obtained from the image processing are validated by comparing the results of physical indices obtained experimentally. Therefore, this work will show the applicability, limitations, and results of analyzes using the aforementioned tools, concluding that as long as there are minimal computational conditions for image processing, the analysis of materials can be done with academic quality and reliability in the public domain.

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MS05 / **917**

Using Low-Field Nuclear Magnetic Resonance and Computed Tomography Imaging to Explore Potential of Ureolysis-Induced Calcium Carbonate Precipitation Treatment to Seal Fractures in Shale

Author: Matthew R. Willett[1]

Co-authors: Kayla Bedey [1]; Laura Dobeck [1]; Dustin Crandall [2]; Johnathan Moore [3]; Jonny Rutqvist [4]; Al Cunningham [5]; Joseph Seymour [1]; Adrienne Phillips [1]; Catherine Kirkland [1]

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[2] *US Department of Energy - National Energy Technology Laboratory*

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Ureolysis-Induced Calcium Carbonate Precipitation (UICP) is an emerging biotechnology which utilizes the enzyme urease to convert urea and calcium into calcium carbonate (CaCO3) deposits for numerous engineering applications. Studies have shown that UICP can be used to seal fractures in shale, raising the possibility of applying this technology to restimulate fracking wells by plugging underperforming fractures. For this and other applications to become a reality, a study is needed to determine how effectively UICP seals shale fractures under subsurface conditions. These fractures constitute a "macroporous"environment in which microorganisms and calcium mineralizing media flow and react between pieces of proppant, though shale itself is an ultralow porous material on the order of nanometers. Thus, it is also of interest to explore if the shale is affected by UICP treatment. Low-field nuclear magnetic resonance (LF-NMR) is a non-invasive approach used to study porosity and pore-size distributions in porous media using the principles of NMR relaxometry. In saturated shale samples, hydrogen nuclei from water trapped in pores and fractures of increasing size have increasingly longer rates of NMR T1 and T2 relaxation. Additionally, shale is rich in organics such as bitumen and kerogen, which have a unique T1 and T2 relaxation signature. Thus, a T1- T2 relaxation correlation can provide insight into the organic and pore/fracture populations within the shale. Tracking how the populations shift after UICP treatment can reveal the extent of biomineralization and may indicate how the organic fraction is affected by UICP. Further insight is provided by X-Ray computed tomography (CT) imaging, another non-invasive technique, which can quantify changes in fracture volume along the length of the core and reveal how CaCO3 is distributed within the fracture. In this study, two-inch long and one-inch wide shale cores with 1-2 mm fracture gap were biomineralized with UICP treatment at 60℃ to mimic subsurface conditions although elevated pressures were not applied. UICP treatment encompassed injection of S. pasteurii microorganisms into the fracture, a brief attachment period, and then an injection of urea and calcium solution, followed by a two-hour batch reaction time. Injections were repeated until three orders of magnitude permeability reduction were measured. This study will present the results of CT imaging and NMR analysis of the biomineralized cores. Non-invasive tools such as NMR and CT help reveal how UICP treatment at elevated temperature affects shale properties and the extent of biomineralization within fractures—and ultimately its suitability for deployment in the subsurface.

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In-Person

References:

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Energy Transition Focused Abstracts:

918

Coreflood Study of Combined Low-Salinity Water and Chemical Process for EOR at Field Conditions in a Reservoir Core

Authors: Teresa Guadalupe Roldán Carrillo[1]; Rodrigo Orlando Salazar Castillo[1]; Gladys Teresa Castorena Cortés[1]; Patricia Olguín Lora[1]

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The scientific community acknowledges the potential of low-salinity water (LSW) to increase the recovery factor in sandstone and carbonate reservoirs (Nande & Patwardhan, 2022; Snosy et al., 2020). LSW injection shifts the wettability of the rock to a water-wet state. It, therefore, promotes the release of additional oil compared to the injection of high-salinity water, such as seawater or formation brine.

On the other hand, many synthetic chemicals are commonly used as EOR agents (Gbadamosi et al., 2019). Depending on their nature, these chemicals enhance oil recovery by either reducing the interfacial tension, altering wettability, or improving sweep efficiency, among other mechanisms.

Combining LSW with chemical injection could be mutually beneficial (Lee & Lee, 2019; Gbadamosi et al., 2022). For instance, LSW reduces the adsorption of the EOR chemical in the rock. Even more, the reduction of the interfacial tension and additional alteration of wettability enhance recovery of the oil left behind by the injection of LSW. This synergy has successfully been tested in coreflood experiments using model rocks (Berea) and model oils (Alagic & Skauge, 2010; Araz & Kamyabi, 2021).

This work assessed the potential of adding a chemical in low-salinity water to increase oil recovery in a target sandstone reservoir. To that end, a coreflood experiment was performed in a sandstone rock from a Mexican sandstone reservoir, using reservoir fluids (crude oil and synthetic formation brine) at a temperature of 114 ℃ and a pressure of 4000 psi.

As the first step, a surface-active chemical was screened at the conditions of the target reservoir. To this end, contact angle and interfacial tension measurements were performed. The selected chemical (C1) can reduce interfacial tension (TIF) and alter wettability to a water-wet state.

The preparation procedure of the core is as follows. A homogeneous reservoir sandstone core was saturated with synthetic formation water (FWs). Then, crude oil was injected until reaching irreducible water saturation. Finally, the core saturated with oil at irreducible water was aged for two weeks at reservoir pressure and temperature conditions.

Three injection fluids were used in this study: seawater (SW), diluted seawater as low salinity water (LSW), and low salinity water with the selected chemical C1 dissolved in it (LSC1).

The injection scheme was performed as follows: SW was injected first to mimic secondary recovery. Once no more oil was produced by SW injection, the tertiary mode was started by injecting the fluid LSW. Again, after oil production stopped, the injection fluid was changed to LSC1. The recovery factor, pressure drop, pH, and ion content of the produced brine were recorded during the experiment.

The two fluids injected in tertiary mode, LSW and LSC1 increased the recovery factor by 6%. This recovery confirms that reducing the salinity and adding the chemical C1 increases the recovery factor in a reservoir core in an experiment conducted at reservoir temperature and pressure. In addition, a core deformation at the end of the experiment was observed. This last phenomenon could be attributed to compression and fines migration.

Participation:

Online

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MS22 / 919

Generating multi-modal pore size distributions for low-density micro-porous carbons using virtual void method in quenched molecular dynamics simulations

Authors: Zhifen Luo[1]; Stephen Burrows[1]; Edo Boek[2]

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The creation and properties of micro-porous carbons are of extreme importance for optimizing the performance of battery and supercapacitor electrodes, as well as vehicular hydrogen storage. In many cases, it is difficult to establish the microscopic structure of experimentally manufactured porous carbons. Atomistic simulation methods with reactive potentials have shown promise to fill this knowledge gap by creating realistic porous carbon structures. However, thus far such models have been unable to reproduce **low-density microporous carbon** structures due to clustering of atoms in high density regions, resulting in a small number of mesopores. Recently, we presented a new method using virtual voids, generating excluded volume by a soft repulsive potential which is progressively decoupled from the carbon atoms (Luo et al., 2021). This allows us to prevent densification and to create disordered carbon models with porosities up to 90%. We vary the size and density of the virtual voids and show that the mean of the pore size distribution and the accessible surface area can be controlled. By choosing the desired porosity and virtual void size, we created amorphous carbon models with mean pore sizes ranging from 10 to 32 Å, which agree favourably with experimental pore sizes for low-density microporous carbons. Our key findings were as follows: 1. Using the traditional quenched molecular dynamics simulation method, we confirm that carbon atoms are likely to accumulate in high density regions, preventing the formation of microporous structures [Ranganathan et al.,2017]. When using virtual voids, the carbon atoms and pores can be distributed uniformly over the whole system to generate microporous carbon with an approximately Gaussian pore size distribution and porosity up to 90%. The addition of virtual voids produced no significant effects on the short-range bonding structure characteristics; 2. Using different sized virtual voids, we gain control over the pore size distribution and surface area of the final structure. A Gaussian function was fit to the pore size distributions, which worked particularly well for smaller virtual void radius. Almost entirely microporous structures, with pore sizes < 20 Å, could be obtained using a virtual void radius of 3-4 Å. At a density of 1 g/cc, mean pore sizes ranging from 10.3 Å to 21.6

Å were found using virtual void radii from 3 Å to 10 Å, respectively. Here we extend our recent work and generate **multi-modal pore size distributions** for low-density porous carbons, using multi-modal distributions of virtual voids. This allows us to make more accurate comparisons with experimentally generated micro-porous carbons, which often have a wide distribution of pore sizes. Indeed, by using a combination of up to three different virtual void diameters, see Fig.1, we are able to create amorphous porous carbon structures with pore size distributions closely resembling experimental results. This enables us to create a comprehensive library of porous carbon structures using our multi-modal virtual void method, complementing the limited number of experimentally generated porous carbons. In turn, this may allow us to design **optimal carbon electrode structures** with respect to electrolyte permeability and carbon surface area.

Participation:

In-Person

References:

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MS06-A / 920

Melting Kinetics of Permafrost under Overlaying Saline Water

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Co-authors: Wei Yang ; Ke Xu [1]

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We experimentally investigate ice melting in porous media under overlaying saline water. Its kinetics provide key information to evaluate the consequences of seawater invasion into permafrost zone caused by global climate change, as melted permafrost may release significant amount of underground methane that further exacerbates the global warming.

Model permafrost is fabricated by glass bead-pack saturated with ice, at the temperature of -5℃. Excessive NaCl aqueous solution initially lays above the model permafrost which further induces melting. We vary glass bead diameter from 0.1-1 mm and salinity up to 25 wt%. Saline water is dyed, so the melting front evolution can be recorded by camera. The fluid system is characterized by its Rayleigh number, $Ra=(k\triangle\rho gH)/(\varphi\mu D)$, where $\triangle\rho$ is the density contrast between overlaying

saline water and the diluted saline water that equilibrates to the ice under the experimental temperature. The melting kinetics is evaluated by the Sherwood number, Sh, which is acquired by image analysis.

Surprisingly, we identify three distinct modes of the melting kinetics, which are governed by the value of Ra (Fig. 1):

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1) The stable mode, in which case the melting front is horizontal and stably moving downward. The concentration of the saline water is uniform, indicating good mixing in the melted zone. This mode emerges when Ra > 1500, namely at high salinity and high permeability.
2) The critical mode, in which the melting front is flat but the concentration of the brine in the melting zone is obviously non-uniform. Typical Rayleigh-Darcy convection can be identified in the melted zone. This mode emerges when 330 < Ra < 1500.
3) The unstable mode, in which case fingers develop at the melting front. This mode emerges at low salinity and low permeability that Ra < 330. We note that this low Ra is very common in practical scenario for seawater invasion into permafrost zone.

We hypothesize that the emergence of these three modes is a result of the interplay between the Rayleigh-Darcy convection and the dispersion kinetics. Stability analysis and numerical simulation validate this hypothesis.

In the context of global warming, the unstable melting with fingering implies that seawater can penetrate down through frozen layer of permafrost much deeper than previously estimated. It thus brings higher risk for underground methane to be released into the atmosphere.

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MS09 / **921**

Multiscale forward modeling of the interplay between carbonate precipitation and porous media transport properties during geological carbon sequestration

Authors: Tianxiao Shen[1]; Shaina Kelly[2]

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Geologic storage of CO2 is a critical decarbonization pathway. CO2 and other fluids are primarily stored through four trapping mechanisms (physical/structural, capillary, dissolution, and mineralization trapping) all of which exhibit spatial-temporal changes throughout a porous material. Controls on the distribution of mineral dissolution and carbonate precipitation and the evolution of porosity and permeability as a function of in-situ and operational parameters is highly multivariate. This research seeks to quantify the effects of early carbonate precipitation on formation CO2 storage capacity, hydrodynamic patterns, and mineralization rate with multiscale forward modeling in several key storage rock lithologies. Here early time refers to a time period on the order of the lifetime of an injection project (~50 years).

We posit that a strategic forward modeling approach using several pore-scale modeling tools and multiple realizations of accessible reactive surface area afforded by high performance computing (HPC) combined with complementary experimental data (feedback-loop) will: (a) elucidate the impact of mineralization for a given range of routine petrophysical properties and (b) provide a framework for upscaling the impact of concurrently investigated reactive transport functional relationships. A combination of pore network models (PNM) and pore-scale computational fluid dynamics (CFD) models are used for digital evaluation of key porous media transport properties that inform a reservoir-scale storage model: cell porosity, permeability, and brine-CO2 capillary pressure-saturation (Pc-Sw) and relative permeability (Kr-Sw). The studied rock types represent a spectrum of porosity, permeability, and reactive mineral surfaces: porous sandstones, volcanic-rich sandstones, igneous and metamorphic rocks (e.g., basalts and serpentinites), and synthetics/composites. This work concentrates on two main injection scenarios, supercritical CO2 injection in deep saline aquifers and dissolved CO2 injection in a mafic/ultramafic formation. The morphological distributions of mineral dissolution and carbonate precipitation (nucleation) are incorporated by way of experimentally-based and theoretical models at the pore scale, determined or benchmarked by reactive transport experiments and pre-/post-reaction characterization and imaging, generated from concurrent in-house and collaborator studies. Pore-scale reactive transport modeling is also used to establish local relationships, where applicable.

In consideration of the heterogeneous nature of geological formations and lithologies, the numerical modeling with the precipitation rules will be applied to multiple 3D representations (informed by routine and special core analysis data and petrographic images) of the selected rock types, and a probability density distribution of the alteration and flow relationships will be established. To demonstrate the impact of the pore-scale findings, the dynamic Pc-Sw and Kr-Sw relationship ranges acquired from the pore-scale modeling processes are upscaled with a reservoir-scale model to show the effect of pore-scale precipitation on storage capacity, hydrodynamic patterns, and the total mineralization ratio of injected CO2 for a selected reservoir geometry and injection scenario. The authors note that the multiscale workflow can be used to determine precipitation pathways for various environmental porous media including surface rocks, mine tailings, and the build environment. Ongoing and future work will include incorporation of controlled fluidic experiments to inform the functional relationships on carbonate precipitation, particularly in complex pore systems such as nanoscale confinements.

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MS13 / 922

Gas and Water Flow Regulations in Remolded Hydrate-hosting Porous Media Based on Non-Darcy Correction of the Pore Network Modeling

Author: Shanshan Zhou[1]

Co-authors: Kunpeng Xue [2]; Guanbin Liu [2]; Tian Xue [2]; Vahid Niasar [3]; Yu Liu [2]

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Natural gas hydrate (NGH) is considered as a type of potential clean energy resource concentrated in permafrost layers and deep ocean floors. The hydrate reservoirs in South China Sea (SCS) have small pore size (0.1 μm -100 μm) and extremely low intrinsic permeability (about 5 mD). and the grains mainly range from clayey silt to silt. Permeability is one of the most decisive parameters in controlling the distribution and concentration of gas hydrate and fluid flow in hydrate-bearing sediments (HBS), which determines the efficiency of gas recovery from hydrate reservoirs.

Due to the extreme complexity of multiphase-flow experiments with hydrate, pore network model (PNM) is widely used to estimate relative permeability. Percolation characteristics simulation results largely rely on the accuracy and feasibility of physical equations in PNM, especially Darcy's theory. The accuracy and feasibility of PNM in simulating the gas and water relative permeability have been proved in the coarse-grained hydrate-bearing porous media. However, in the fine-grained sediments, numerous researchers have found that gas and water flow mechanisms is away from Darcy's theory-the basic theory of the PNM.

In this study, mercury penetration experiments were firstly conducted to obtain pore size distribution of Berea sand and remolded hydrate-host sediments from SCS. Next, we made a criterion of the gas flow regime in these two groups of sand based on the Knudsen number. In the following, Darcy equations in the PNM code was modified based on the non-Darcy flow regime. After that, three-dimensional pore networks were extracted from nano X-ray CT images of these two sand samples. And then, based on the extracted pore network, gas and water flow simulation were conducted by PNM with both original Darcy theory and the corrected no-Darcy function. At last, comparisons were made between the two-phase flow relative permeability results calculated by original and the corrected Darcy function to judge the gas and water relative permeabilities variation.

Results showed that gas-slip effect occurred in remolded hydrate-host sediments. Both gas and water relative permeabilities at the same water saturation calculated by the corrected PNM code with No-Darcy function were lower than those calculated by the original PNM with Darcy theory. Results showed that the PNM used in low-permeability natural gas hydrate reservoir is essential to be calibrated by non-Darcy theory function.

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The effects of sand bridge structures on gas and water relative permeability evolution during the continuous sand migration process in hydrate-bearing porous media

Author: Shanshan Zhou[None]

Co-authors: Kunpeng Xue [1]; Tian Xue [1]; Guanbin Liu [1]; Yu Liu [1]; Vahid Niasar [2]

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Natural gas hydrate is a type of potential clean energy resource with vast reserves concentrated in the permafrost and submarine deposits as a solid phase. During the hydrate exploitation process, the hydrate transforms from a solid phase to the gas and water phases and flows in the porous media. Particle movement occurs in the pore space due to the hydrate phase transition, leading to the variation of gas and water flow.

In this study, Micro X-Ray Computed Tomography (CT) and a pore network model (PNM) were adopted to study gas and water flow during a continuous sand migration process in hydrate-bearing porous media. First, the continuous hydrate dissociation experiment was conducted in the hydrate-bearing sample with an optimal median grain size ratio (6.5) under conditions of a thermal-stimulated process. Then, four groups of CT images were obtained and used to visualize the 3D pore network. Next, pore space parameters are calculated after image processing. After that, gas and water flow were analyzed by the PNM.

Results showed that in the early stage, the increase of pore space connectivity expansion caused by hydrate dissociation was the main factor in gas-water flow increment. With the continuous hydrate dissociation, the sharp increase of tiny pore and throat numbers caused by sand bridge structures were the main factors leading to the decrease of both gas and water relative permeability. At the final stage, sand migration and gas and water flow were mainly influenced by the occurrence of stable sand bridge structures. Moreover, gas and water relative permeabilities at the same water saturation were larger than that in the initial stage. And the extension of the pore space caused by hydrate dissociation was in charge of this result. Sand bridge structure in controlling gas and water relative permeabilities in this study can be considered as a micro mechanism reference in considering both sand production and fluid flow ability in hydrate-bearing porous media under the process of hydrate dissociation.

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Poster / 924

Effect of Water on the Methane Adsorption on the Na-Montmorillonite Surface: Molecular Dynamics Study

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The study of methane adsorption on the surface and in the interlayer space of clay minerals is of great importance for the exploration and production of natural gas and shale hydrocarbons. Substantial part of the shale gas exists in the adsorbed state, so understanding the adsorption capacity as well as mechanisms of adsorption is important to properly estimate the amount of shale gas and to develop recovery strategies. Humidity is one of the key factors influencing gas adsorption. The goal of this work is to study the effect of the water coverage of a weakly charged clay mineral in slit-like pore on methane adsorption by the molecular dynamics method. An atomistic model of montmorillonite with the structural formula $Na_{0.75}(Al_{3.75}Mg_{0.25})(Si_{7.75}Al_{0.25})O_{20}(OH)_4 \cdot 2.5H_2O$ was used as a surface model. The interaction between the clay mineral, metal ions, and water molecules was described by the ClayFF force field. The methane molecules were described by Trappe-UA and OPLS-AA models. It was shown that the choice of the force field has little effect on the results. At STP conditions methane molecules adsorb at the centers of free siloxane rings on the surface and water molecules do not affect the adsorption mechanism.

As higher pressures (>6 MPa), two peaks are observed in the methane density profile, indicating the presence of two methane adsorption layers near the pore walls. The first adsorption layer is always ordered and contains methane even with high amount of H_2O molecules. The structure of the second adsorption layer depends on the pressure and amount of water.

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926

Porous Media as Active Matter for Future Energy Supply and Climate Remediation

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Current projections of the future energy consumption propose a radical reduction of conventional energy use and that sustainable extraction of critical minerals should supply raw materials for renewable energy. With the global decline in the discovery rates of new mineral deposits, minimising the energetic costs for processing minerals and metals is crucial to reducing the carbon footprint and vital for the economic success of operations. For example, in mining, the comminution of raw ore is the most significant energy sink. The energy consumption of the industrial process depends significantly on the original material microstructure. Computational models of the coupled multi-physics processes underpinning the relevant manufacturing steps constitute an indispensable tool for optimisation in process, material, and energy extraction.

There are three challenges. First, the underlying coupled thermal, hydro-mechanical, chemical, and electrical (THMCE) multi-physics processes are complex and often poorly understood. Second, the solution of the coupled systems of partial differential equations (PDEs) is mathematically and computationally challenging, and third, direct microstructural observations of dynamic processes in the deforming porous medium are occluded to the observer.

To solve these challenges, we combine a new nonlocal multi-physics wave-mechanics theory to harness the energy stored within the microstructure of solids by activating micro-macro-scale feedback processes. We hypothesise that, by activating these feedback loops, we can turn raw materials into active matter where a thermodynamic force can synergistically trigger a thermodynamic flux of another kind. Recently, the study of such active matter in biological, biopolymers, colloidal systems, and artificial particles gained significant momentum. Active matter, driven far from equilibrium on its microscale, displays unexpected behaviour by local dissipation of internal energy under an external forcing, for instance, displaying self-propelled motion and self-assembly. Under the right conditions, an external load can sustain "perpetuum-mobile-like"behaviour. For a constant load, while internal (microstructural) energy is available, the motion continues; otherwise, it stops.

Active matter involves chemical or fluid and mechanical mass fluxes to be unbalanced locally such that no effective stress principle applies. It allows consideration of the possible interdependence of solid pressure fluxes through matrix deformation enabling dehydration reactions for fluid release mass fluxes in a nonlocal diffusive region. This interdependence can cause the local fluid pressure to go through rapid changes accompanied by enforced mass exchange with the matrix environment in the highly pressurized mixture. Such systems are understood as an entangled system in which classical physics fails to describe the additional the capacity to tunnel through an energy barrier through nonlocal interactions as in catalysts.

Here we discuss a promising application of the new approach. Novel breakthrough catalysts which facilitate energy conversion or CO2 adsorption reactions have already been developed for renewable energy in the laboratory scale. However, they are extremely delicate. Upscaling to a porous 3-D network to achieve maximum surface for catalyst reaction without losing stability under operational loads is crucial. A potential future breakthrough for use of the catalysts is their capability to operate synergistically with the applied environment by unlocking a larger scale tunnelling effect up to the system size.

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927

Typical elements recognizing and morphological characteristics assessing of air voids in asphalt mixture

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Air void is the primary passageway for water infiltration in asphalt pavements. Its morphological characteristics and structure framework directly impact the inner water transfer behavior and further decide the pavement performance in a water environment. However, the existing void analysis method ignored the complicated void structure and failed to recognize the typical void elements, which allows the research gap in assessing the effect of void structure on micro water transportation.

In this study, the digital processing based on X-ray CT images was conducted on three types of asphalt mixture, including asphalt concrete (AC), stone matrix asphalt (SMA), and open-graded friction concrete (OGFC). The digital void model which consisted of the slices and frameworks was developed. The evaluation indexes, including plumpness, roundness, frame angle, and vertical plane angle, were established to assess the morphological characteristics of voids. After a comprehensive investigation of the void slice and framework property, the typical elements consisting of the vertical throat, corridor throat, tank, cone branch, and structured branch, were proposed. And the typical void elements recognizing algorithm was developed.

The results show that the frame angle and vertical plane angle show superiority in the large angle region in AC, indicating the void frameworks in AC are more tortuous than SMA and OGFC. The roundness and plumpness of the void slices in OGFC are higher than that in the other two asphalt mixture types, which concludes the voids in OGFC are relatively regular among the three types of asphalt mixture. With regard to the typical elements, the proportion of the tank in OGFC is 15~20 % higher than that in AC and SMA, which indicates the void structure in OGFC contains extensive large volume units for water storage. While the proportion of the vertical throat and corridor throat in OGFC is lower than the other two asphalt mixture types. The proportion of the throat reaches 64 % in SMA, and 55 % in AC. This phenomenon indicates that it has more resistance for water seepage in SMA and AC. In addition, the roundness and plumpness of the void throat in SMA are higher than that in AC. While the vertical plane angle in SMA is lower than that in AC. That indicates the framework of the void structure is straighter and the void slices are more regular in the throat of SMA than in AC.

The result contributes to understanding the effect of the separated void structure on water transportation behavior and proposed a method to recognize the typical elements of void in asphalt mixture.

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Energy Transition Focused Abstracts:

929

A thermal-poro-elasto-plastic coupled model of hydraulic fracturing in deep reservoirs

Authors: Wenzheng Liu[1]; Wenzhong Li[1]; Yuanpeng Jiang[1]; Yu Wang[1]; Jianting Huang[1]

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With the rapid growth in the global demand for oil and gas resources and the successful development of middle–shallow formations, the exploitation of oil and gas reservoirs is gradually extended to deep formations. Hydraulic fracturing is a key technology for successful development of deep reservoirs. However, the production of deep reservoirs faces the problem of "three highs"(high temperature, high pressure, and high in-situ stress), resulting in the transformation of rock mechanical properties from elasticity to plasticity. The hydraulic fracturing process in deep reservoirs involves complex multi-physical effects, and the rock mass may exhibit extensive plastic deformation. The prevailing fracture propagation models based on the linear elastic fracture mechanics are no longer applicable to predict the evolution process of hydraulic fractures in deep formations. In this work, considering rock plasticity and thermal-hydro-mechanical coupling, the mathematical models of hydraulic fracture propagation in deep reservoirs are established based on elasto-plastic theory, Biot's theory, local non-thermal equilibrium theory and cohesive zone model. The FEM and return-mapping method are used to simulate the deformation of inelastic media with strong discontinuities. The discontinuous pressure field and temperature field is simulated by the DFM and FVM. In addition, a dual-layer iterative algorithm is proposed to solve the strong nonlinear systems by a combination of the fixed-stress iteration, Picard iteration and Newton-Raphson iterative method. Then, the accuracy and ability of the proposed model are demonstrated through several reference cases. Finally, the proposed model is applied to investigate the propagation mechanism of hydraulic fracture under thermo-poro-elasto-plastic coupling. Results show thermal stress generated by the temperature difference between fracturing fluid and rock can reduce fracture extension pressure, and cooling effect can reduce the adverse effect of rock plasticity on hydraulic fracturing. In addition, the increase in fluid temperature during the fracturing process leads to a decrease in viscosity, which can also reduce fracture extension pressure.

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930

Nonlocality stemming from dynamic interaction between the skeleton, the pore, and the environment

Authors: ManMan Hu[1]; Klaus Regenauer-Lieb[2]

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A nonlocal approach here considers the microscopic interaction between skeleton and pore fluid in an integrated way where the fluxes of both constituents are not bounded by the local equilibrium assumption. Mass balance is achieved at the Representative Elementary Volume (RVE)-scale which leads to the identification of new reaction and diffusion terms, here called cross-reaction and cross-diffusion. These terms appear in addition to the self-diffusion process of the macroscopic system described by local theories. We propose that they are key to pattern forming processes. Here we apply a reaction-diffusion formalism extended by nonlocal cross-diffusion/reactions terms for poromechanical processes and resolve additional system dynamics on shorter time and length scales that have been overlooked. We argue that these processes are crucial for understanding the pathway to instabilities of fluid-filled porous media and can alter the overall system behaviour in response to the environment. This is hence essential for forecasting efforts of instabilities. For the overall system response, it is necessary to identify situations for possible triggering of extreme events. These were previously not captured since the cross-reaction/diffusion processes are assumed to have relaxed to local equilibrium in classical theories.

Here we discuss one example (a natural geomaterial) where nonlocal interactions between the skeleton, the pore fluid and the environment are triggering large-scale instabilities. We consider a subducting slab where the hydrated mineral serpentinite starts to break down at a given temperature during the plunge of the slab into the earth's mantle. The mineral breakdown occurs only when there is space for the fluid to flow thus requiring a porous environment. Serpentinite itself is, however, a very tight formation and cracking (or local phase separation) is required to form the voids where the fluid can flow into. This interaction is highly dynamic and cannot be described by a classical self-diffusion formalism, while the nonlocal length and time scales become prominent. There are two representative dynamical scenarios caused by these nonlocal interactions.

The first is a perfectly periodic long-time scale (multiple months) chemo-poro-mechanical oscillator where a fast silent slip event is triggered by release of the internal energy of the geomaterial through an exothermic reaction and fluids are generated inducing hydrofracturing, followed by slow creep where the subduction process provides mechanical work to facilitate the endothermic rehydration reaction. This phenomenon has been recognised in many subduction environments through GPS recording of episodic oscillating silent slip. The fast dehydration branch is accompanied by seismic tremor interpreted to be the consequence of the volume change. The term Episodic-Tremor and Slip (ETS) has been coined to describe this fundamental thermodynamic oscillator.

The second dynamical scenario is a globally synchronised "violent"serpentinite dehydration event that occurs when the cross-diffusion phenomenon takes short time-scale control over the subduction process. During this event the exothermic processes are working in unison creating mechanical work and providing a possible trigger for a major earthquake (as recorded 12 times over the past 6700 years in the Cascadia subduction zone) which is considered the archetype of silent subduction systems underlined by ETS cycles.

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Poster / 931

Expanding Digital Rocks Portal with benchmark datasets and engineered porous media

Author: Masa Prodanovic[1]

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Digital Rocks Portal (DRP, https://www.digitalrocksportal.org) organizes and preserves imaged datasets and experimental measurements of porous materials in subsurface, and beyond, with the mission to connect them to simulation and analysis, as well as educate the research community. We have over 150 projects represented in more than 200 publications, and an active community that reuses the data, most recently in multiple machine learning applications for automating image analysis as well as the prediction of transport. Such automation is crucial for performing formation evaluation tasks in near-real time. We present benchmark datasets that have played a role in recent machine learning prediction successes in the field. We further discuss the vision for further research advances, educational materials, as well as growth and sustainability plan of this digital rock physics community resource. In particular, we are in the process of expanding into a broader repository of engineered porous materials, specifically those for energy storage and the portal will transition to Digital Porous Media (DPM) in near future.

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MS08 / **932**

Rayleigh-Darcy convection in a three-dimensional granular medium: an experimental study

Author: Shabina Ashraf[1]

Co-authors: Jaybrata Dhar [2]; Francois Nadal [3]; Patrice Meunier [4]; Yves Méheust [5]

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The reduction of atmospheric greenhouse gas concentrations, for which CO2 contributes to 70% of the greenhouse effect, involves securely trapping CO2 in the subsurface. This is done by one of the four main mechanisms, namely structural, residual, dissolution, and mineral trapping [1-3], in the order of their storage security. Dissolution trapping in deep saline aquifers occurs when the supercritical CO2 trapped below the cap rock dissolves into the brine underneath. The CO2-enriched brine has a higher density than the ambient aquifer fluid, which causes it to form a gravitationally-unstable layer between the pure brine and the supercritical CO2. This unstable layer's destabilization develops into a natural convection that brings the dissolved CO2 to the lower regions of the aquifer while providing fresh brine to the brine-supercritical CO2 interface, in which the latter can further dissolve [4,5].

This convective dissolution of CO2 in a brine saturating a granular porous medium was recently investigated by Brouzet et al. [6] using refractive index matching and planar-laser-induced fluorescence. In their study, the growth dynamics of the instability was significantly different from Darcy-scale theoretical predictions. They explained this discrepancy by the coupling of heterogeneous advection and solute mixing at the pore scale, which cannot be accounted for by Darcy scale models, unless they take local porosity fluctuations into account. These results suggest that Darcy scale models of convective dissolution may underestimate the typical time scale of dissolution trapping by up to several orders of magnitude.

In line with the work of Brouzet et al., we focus here on experimentally chacterizing the Rayleigh-Darcy instability and resulting convection inside a three-dimensional (3D) granular porous medium. That is, we decorrelate the convection from the dissolution, and use analog fluids to study the former alone. The miscible light and heavy analog fluids'(solutions of Triton X-100, water, and zinc chloride) refractive index is matched to that of the porous medium's transparent PMMA grains, to render the medium transparent. The density difference between the fluids is achieved by adding a different amount of ZnCl2. The heavier fluid initially carries a uniform colouring dye (Nile blue) concentration. We control the Rayleigh (Ra) number quantifying the initial strength of the instability, and the Darcy number (Da) quantifying the model aquifer's vertical size by changing the densities of fluids and the size of the grains. A custom-made optical tomography scanner is used to reconstruct the 3D dye concentration field from horizontal cross-sections. The convection dynamics are analyzed from the growth rate of the fingers and the finger number density. Measurements are performed for various values of Ra, andand, independently, for each of them, for various values of the number

Ra√Da, which quantifies the typical size of the most unstable instability mode with respect to the typical pore size. The results seem to be consistent with the findings by Brouzet et al.

Participation:

In-Person

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Poster / 933

The impact of heterogeneity in the pore structure of a laboratory sedimented clay sample when measuring swelling anisotropy

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This study sets out to investigate the anisotropy of clay swelling by comparing the free swelling of specimens sampled radially and axially at different location in a large laboratory sedimented clay sample 20 x 6cm (diameter x height). The free swelling was measured on 2 x 2cm (diameter x height) cylindrical specimens sampled with stiff plastic containers having a closed based. The base had a small hole to allow air to escape during the sampling process and a filter paper was position at the base to allow uniform hydraulic boundary conditions during swelling. The sample was then placed in the chamber of a H1 Nuclear Magnetic Resonance setup and porosity was assessed through interpretation of the transverse relaxation time (T2) spectra. In addition, the setup used also provides the water profile along the sample, which allows to study the uniformity of the pore structure before and during swelling. Swelling was induced by filling the chamber with deionized water that entered the specimen from the base of the sampler. The porosity and water profile were then assessed at different time intervals and once marginal changes were observed the specimen was removed and the free swell was additionally measured with a gauge. Specimens taken both in the radial and axial

direction were compared, as well at different distances from the center line and the sample faces. The results therefore address two issues related to homogeneity: the extent of initial pore structure homogeneity in a large laboratory sedimented sample and the homogeneity in swelling of the pore structure; besides swelling anisotropy due to preferential clay particles orientation during sedimentation.
The preparation of resedimented artificial soil samples is a common practice in geotechnical laboratory in many instances. Firstly, this may be applied to an intact sample (i.e. either block or core samples) for removing its structure, defined here as the combination of particle bonding and fabric. The aim being to quantifying the effects of such structure by subsequent comparison of the mechanical behaviour of the two samples (e.g. Burland 1990; or Cotecchia & Chandler 2000). Secondly, this technique has been widely used to prepared specimens for mechanical testing of those soils too difficult to sample without significant disturbance. Most commonly mine tailings, soil mixtures and intermediate soils, which tend to liquefy during sampling. In particular, Carraro & Prezzi (2008) devised a method to be employed for the preparation of individual specimens, while others (e.g. Shipton & Coop 2015) opted for batch production by using a large consolidometer to obtain a large "cake"to be then subsampled. Such technique is also typically chosen when artificial mixtures are prepared for ease and speed of production, e.g. when investigating fundamental aspects of soil behaviour. The possible separation of components during the sedimentation process is of particular concern in the case of soil mixture as this might result in heterogeneous samples. However, it has been observed also when resedimenting "pure clay"samples (Stallebrass et al. 2008).

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

934

Optimizing the sweep efficiency of injection fluid in a waterflooding process with Reinforcement Learning

Authors: Bineet Kumar Tripathi[1]; Indrajeet Kumar[1]; Anugrah Singh[1]

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Due to the complex and unpredictable dynamics of the waterflooding, optimization of oil recovery in closed-loop management is always a difficult problem to solve. To maximize the total oil produc-

tion, optimization of waterflooding using model-free reinforcement learning (RL) can potentially increase the sweep efficiency of injection fluid. However, previous studies based on dynamic optimization, such as nominal optimization, reactive-control approach, etc., often lack robustness in the reservoir uncertainties. The presence of parametric uncertainties (like reservoir permeability, porosity, wettability, etc.) can significantly reduce the recovery from the reservoir. These uncertainties create problem for well control and reservoir management. In this study, we propose three model-free RL approaches - proximal policy optimization (PPO), advantage actor-critic (A2C), and deep deterministic policy gradient (DDPG). Tenth SPE Comparative Solution Project (SPE-10) waterflood is a well-known and widely used reservoir case study, which is used to implement and assess the proposed methodology. The saturation and pressure of well at various locations act as the states in the RL formulation for optimizing well control, and the valve openings serve as the actions. The reservoir permeability field is the uncertain model parameter, and the numerical reward is mapped to the overall sweep efficiency. We have optimized the productivity of a 5-spot pattern by using the proposed RL approaches. The results are compared with the differential evolution algorithm and found the RL algorithms to be efficient and robust in optimizing the waterflooding process.

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Poster / 935

Hydrochemically detrimental factors in ATES applications –An analysis of clogging and scaling processes based on column and batch experiments

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Co-authors: Alireza Arab ; Martin Binder ; Christian Engelmann ; Traugott Scheytt

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Aquifer systems represent the major source for mankind's drinking and irrigation water demands. Throughout the past two decades, they have also increasingly got into focus for geothermal energy usage. The protection of groundwater against detrimental impacts is essential to prevent or minimize risks associated with contamination, water scarcity, and to ensure a sustainable transition towards green energy. Together with issues related to the energy production itself (e.g. changing wind abundance at wind parks leading to temporally unstable electricity supply), a large variability of industries temporally as well as seasonally creates surpluses of energy. These surpluses are typically not directly used (e.g., steelworks releasing heat into the atmosphere), which raises needs for (over-)seasonal energy storage capacities to compensate supply-demand ratios.

The BMBF-funded research project 'UnClog-ATES'investigates one of the most common types of storage systems, the so-called 'aquifer thermal energy storage'(ATES) concept. With ATES, thermal energy is intentionally stored underground for a later use. This can be done, for instance, by extracting groundwater during the summer period from the 'cold'well for cooling by using a heat exchanger, and subsequently injecting the heated groundwater directly back into the aquifer to be stored for heating purposes in the winter period. Borehole heat exchangers or (abandoned/partially flooded) underground mines (see sister project 'MineATES') can also be used as parts of such energy storage systems.

In the context of most existing ATES applications, elevated pressure and temperature conditions can lead to unwanted mineral reactions, dissolution and chemical precipitation processes, flocculation, or microbial growth, overall causing clogging and scaling. Among other factors such as rock heat properties or available porosity, an adequate hydraulic permeability of the aquifer matrix is crucial for successful ATES application . The aforementioned processes can hamper its proper functioning, leading to decreasing aquifer permeability and increasing costs for, among others, cleaning clogged pipes and replacing corroded parts. Clogging and scaling processes are to be deeply analyzed in Unclog-ATES, and technical countermeasures (e.g., scaling inhibitors, acids, or CO2) are to be identified with an interdisciplinary consideration of microbiology, geology, hydrogeology and geochemistry.

In the study presented here, we give an overview on influencing factors associated with clogging and scaling in carbonate and silicate aquifers by employing a series of laboratory-scale experiments under defined conditions mimicking typical ATES conditions (pressure, temperature, hydraulics, and chemical composition). In specific, quasi-1-D column setups imitating the transport conditions in the aquifer and, in parallel, batch experiments with intentionally varying chemical milieus and rock compositions, will serve for analyzing possible hydrochemical reactions and precipitation processes as wells as their impact on the system. Expected results of the UnClog-ATES project are predictions for biogeochemical reactions, estimations on the clogging potential and the assessment of possible countermeasures.

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936

Modeling and simulation of chemical reactions in porous media

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Chemical reactions play a key role in the synthesis of specific substances, the removal of harmful substances from mixtures, or in geochemical processes. Due to the increasing need of energy- and resource-efficient processes, the optimization of such processes is an important step. High yield and selectivity are desired. To identify optimization potentials, modeling and simulation is a suitable tool to assist the process development. Reactive transport in porous media is a complex interplay of flow, mass, and energy transport. The first step toward achieving such an optimization task is the development of efficient algorithms for pore scale simulation in the case of complex reactions.
A chain of different software tools is utilized to resolve the chemical reactions enhanced by a catalyst. The central component of this chain is the software tool PoreChem. With this tool, the convective and diffusive transport in the porous medium and the chemical reactions are simulated. Moreover, it is also possible to simulate the temperature distribution and its change due to heat of reaction or external sources. The temperature, on the other hand, influences the reaction rate and therefore also the performance of the reaction. Since the microstructure is resolved, the influence of the specific geometry features on flow, mass, and energy transport can be investigated. In the case of complex catalytic reactions, the choice of the reaction time scales is challenging.
In this presentation, several applications are investigated, e.g. packed bed reactors and catalytic filters. Using simulation, it is shown how the interplay of the geometry, different transport mechanisms, and the chemical reactions influence the outcome of the process.

Participation:

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Energy Transition Focused Abstracts:

MS01 / **937**

Mineral Carbonation Sensitivity to Hydrogeologic Heterogeneity of Basaltic Aquifers

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Co-authors: Benjamin Tutolo [2]; Rachel Lauer [2]; Kong Xiang-Zhao [3]

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Atmospheric CO2 concentrations are expected to double over the next three decades, and reducing its emissions alone will not be enough to reduce greenhouse gas emissions and limit anthropogenic warming. The removal of large quantities of CO2 from the atmosphere or the prevention of newly produced CO2 from reaching the atmosphere is possible through the combination of carbon mineralization in basalt-hosted hydrogeologic systems with direct air or point source capture technologies. Recent efforts in this direction have shown that rapid mineralization is possible, ensuring the security of underground CO2 storage. However, predicting how far the injected CO2

will migrate and how fast it will mineralize as it encounters spatial heterogeneity in basaltic formations presents unique challenges to its full-scale implementation. Previous carbon sequestration research, particularly in sedimentary rocks, has commonly investigated the effects of heterogeneity on CO2 migration, density-driven convection, dissolution efficiency, formation injectivity, and leakage potential. Nonetheless, the efficiency of CO2 conversion to carbonate minerals in heterogeneous basaltic aquifers remains underexplored. In this study, we present our recent efforts to constrain mineral surface area in laboratory experiments with the goal of improving predictions of mineralization and evaluating its combined impacts with heterogeneity at the field scale. A combination of gas sorption measurements, Raman spectroscopy, and backscatter electron imaging (500 nm/pixel) with image processing techniques was utilized to quantify mineral-specific surface areas. We developed a continuum-scale reactive transport model based on these measured surface area values and showed that predictions based on mineral-specific quantifications of surface area are in reasonably good agreement with effluent chemistry produced from CO2 flow-through experiments. While mineral surface area and porosity remain fixed, a spatially varying 3D permeability field, defined by the Dykstra-Parsons coefficients and correlation lengths, introduces heterogeneity to basaltic formations. We systematically generated an ensemble of 100 simulations and computed the mean mineralization efficiency and corresponding correlation of variation in efficiency to analyze the interplay between heterogeneity and the gravity-viscous ratio. Our findings show that variability in permeability yields a greater interfacial area between free-phase CO2 and formation fluids and thereby facilitates its enhanced transformation to carbonate minerals. In this context, we demonstrate that, despite the uncertainty in heterogeneity and the inability to represent heterogeneity at an adequate scale in most numerical models, variability in permeability can enhance carbon mineralization in basaltic aquifers, which has the potential to significantly reduce the global anthropogenic CO2 budget and contribute to the achievement of an energy transition future.

Participation:

In-Person

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MS01 / **938**

Experimental investigation of CO2 dissolution in Ca2+ rich aquifer with precipitation reaction

Authors: Shuai Zheng[1]; Ke Xu[1]

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After CO_2 is sequestrated into deep saline aquifers, it dissolves into underlaying brine. In presence of Ca^{2+}, extensive precipitation reaction may emerge. However, how precipitation reactions impact CO_2 dissolution kinetics is still an open question that affects the evaluation of sequestration safety and efficiency. Three mechanisms are possible: (1) suspended particles changing fluid rheology;

(2) cloudy suspension clog the throats and thus change porosity and permeability; and (3) particles absorb on grain surface thus reduce the in-situ fluid density. Experiments are needed to find the correct mechanism.

We thus conduct visualized experiments in a high-pressure chamber. Calcium hydroxide ($Ca(OH)_2$) solution saturated in bead-pack is positioned into CO_2 atmosphere under 1Mpa, 25 ℃. $Ca(OH)_2$ concentration is one order of magnitude lower than the saturated CO_2 concentration, that reproduces the ratio in practical scenarios. Permeability is tuned over five orders of magnitudes. pH indicator is added into the liquid to enhance visualization.

In all experiments, we observe sharp front where pH quickly transients from 5 to 10, indicting a stable reaction front. It is rationalized by the non-monotonic vertical density profile during the reactive dissolution that the minimum density is at the reaction front. However, the behaviors of precipitation in bulk and in porous media are fundamentally different:

- In bulk, $CaCO_3$ particles are observed as cloudy suspension, that flows with the Rayleigh-Taylor convection. In modeling such scenario, precipitation reactions affect the convection mainly by changing the fluid rheology.

- In porous media, however, NO flowing $CaCO_3$ particles or pore-blocking are observed. In-situ microscopic experiments show very few $CaCO_3$ particles exist, which all absorb on glass bead surface and then re-dissolve (Figure 1(a)). In this case, precipitation rarely affects permeability and porosity; however, as $CaCO_3$ particles no longer flow with fluid, the fluid density at the reaction front is significantly reduced compared to $CaCO_3$ suspension, that affects the convection kinetics.

We further quantitively record the reaction front velocity (U) and correlate it with permeability (k). We find the dissolution kinetics in high and low permeability media are remarkably different: in low perm regime, the U is proportional to k; while in high perm regime, a sublinear U - k dependence is observed that U approximates to a maximum value. We hypothesize that this transition is shaped by 1) dominance of inertia term at large k, and 2) enlarged fluid density contrast due to particle absorption. The transition point is theoretically predicted, and numerical simulation results supports our hypothesis (Figure 1(b)).

This work presents experimental evidence that $CaCO_3$ precipitation may not cause clogging or suspension flow in porous media during CO_2 sequestration. Instead, precipitation reactions in pore structure accelerate CO_2 dissolution rate, by limiting precipitated $CaCO_3$ in pore geometry and on grain surface, thus reshaping the in-situ fluid density which affects the buoyancy-driven convective dissolution kinetics. It thus helps to correctly simulate CO_2 convective dissolution during its subsurface sequestration.

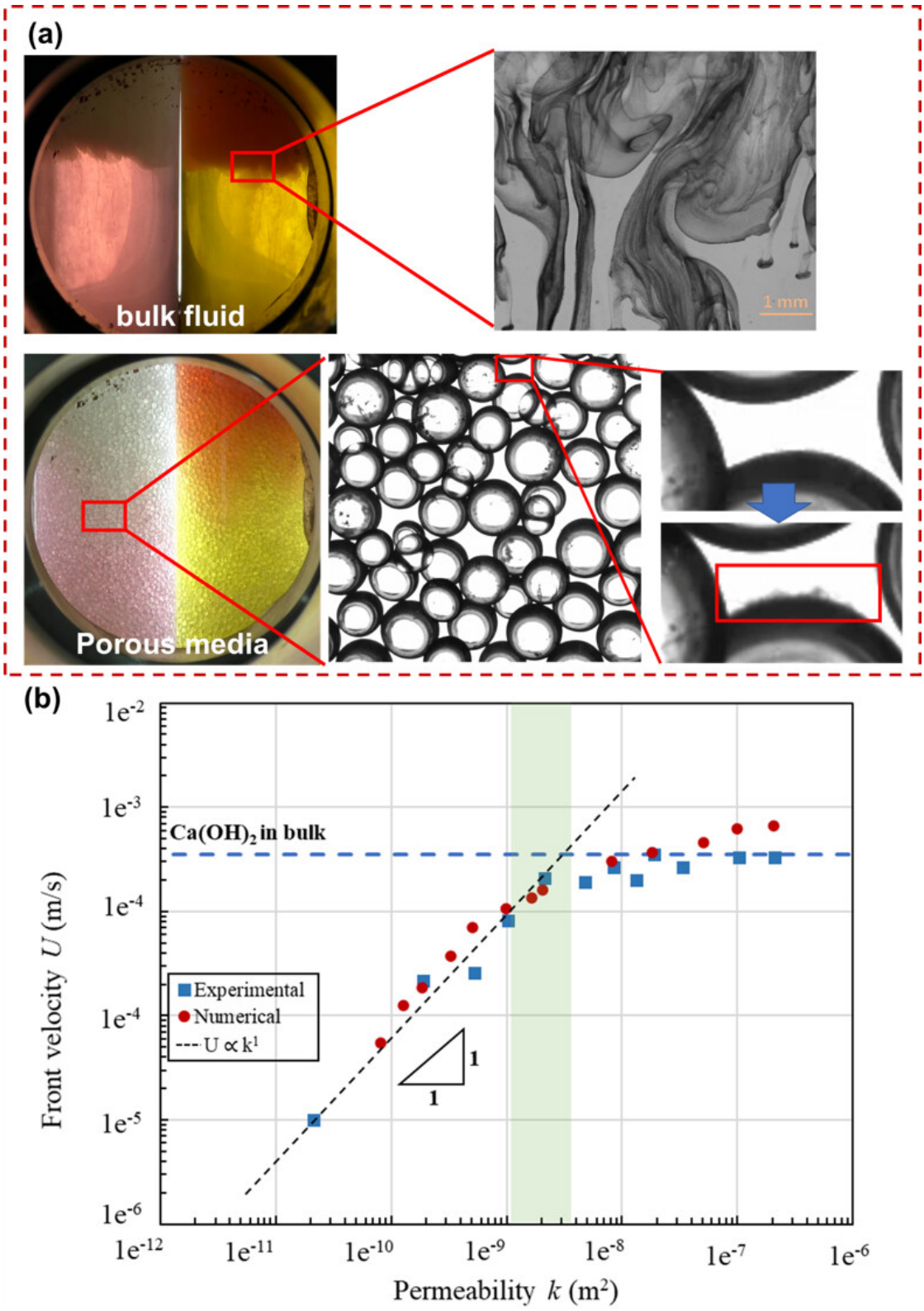

Figure 1: (a) experimental images in bulk and porous media with corresponding microscopic observations; (b) U-k correlation curves obtained from experiments and numerical study.

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Energy Transition Focused Abstracts:

MS09 / 939

Thermodynamic properties of ganglia in heterogeneous porous media

Authors: Chuanxi Wang[1]; Ke Xu[1]

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Ganglia (bubbles, or droplets) are widespread in porous media of various industrial applications. Thermodynamic properties of a ganglion, such as its morphology, free energy, capillary pressure, surface energy, etc., are crucial in determining its transport and reactive performance. Although these in homogeneous porous media have been recently resolved [1, 2], it is still challenging to quantitatively describe the thermodynamic properties of ganglia in heterogeneous media [3-5].

We develop a pore-scale numerical algorithm for determining the thermodynamic properties of hydrostatic ganglia in heterogeneous porous media. We track cycles of quasi-static growth and quasi-static shrinkage of a ganglion in a two-dimensional heterogeneous porous media, as shown in Figure.1(a). The algorithm is as follows:
(1) Create a heterogeneous porous medium and set the initial capillary pressure (Pc) and pore occupancy of the ganglion.
(2) Find the hydrostatic morphology of the ganglia with set Pc and pore occupancy, and record its properties including ganglion volume (V), free energy (F), surface area (A), etc.
(3) Make a small change in Pc while keeping pore occupancy unchanged, and then check whether a new hydrostatic morphology can be achieved. If so, the change is reversible and we go back to step (2) and continue. If not, an irreversible event emerges that changes pore occupancy while keeping V unchanged, and we search for the new stable morphology.

This algorithm may be used to simulate degassing and dissolution process in heterogeneous porous media and enhance our understanding of these processes. In addition, this algorithm may be used to construct the energy landscape of the entire heterogeneous porous media. We believe that this work helps better understand the behaviors of the dispersed phase in heterogeneous porous media.

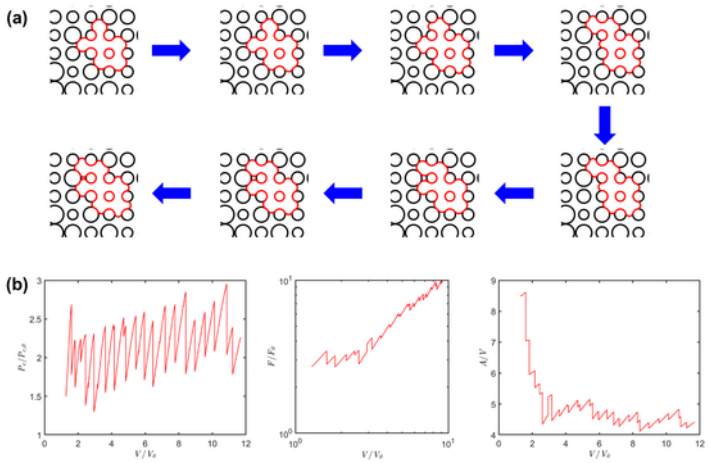

Figure 2: (a) Snapshots of ganglion growth in heterogeneous porous media. (b) Evolution of the capillary pressure, surface free energy, and specific surface area with ganglion volume during ganglion growth in heterogeneous porous media.

Participation:

In-Person

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Energy Transition Focused Abstracts:

940

Experimental Study of Gas Flow in a Nanoporous UK-Based Shale Core Sample

Authors: Hosein Doryani[1]; Mahmoud Jamiolahmady[2]; Jingsheng Ma[3]; Jim Buckman[3]

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Unconventional reservoirs play an important role in the path towards clean energy transition and future energy demands. Several mechanisms are involved in the flow of fluids inside porous media with nano-pores which require accurate experimental and analytical evaluation that need to be understood properly. Among different parameters, gas flow in shales is highly dependent on pore pressure and net stress. During the production from an unconventional reservoir, two simultaneous phenomena would occur. First, pore pressure decreases which results in an increase in gas slippage effects. As a result, measured apparent gas permeability increases. On the other hand, by production from the reservoir, net stress which is the difference between pore pressure and confining pressure increases. As a result of this latter phenomenon, the size of the pores reduces which in turn causes the measured permeability of the gas to reduce. In order to quantify the simultaneous impacts of such phenomena, it is required to have reliable experimental data, especially for shale reservoirs in the UK for which there is very little accurate data available.

The objective of this study is to implement a newly proposed methodology to take into account the effects of pore pressure and net stress in a UK-based shale core sample. Based on our methodology, several systematic pressure pulse decay (PPD) experiments were designed and performed at 50C using an in-house core flooding experimental set up especially designed for measuring the properties of ultralow rock samples at high temperature and high pressure. Gas permeability of the shale sample was measured at various pore pressure values ranging from 250 psi to 4500 psi for a constant net stress of 500 psi. In another set of experiments, at constant pore pressure of 1500 psi, gas permeability was measured at various net stress values ranging from 500 psi to 4000 psi by modifying the confining stress.

The results showed that there are two different regions with time, i.e. early and late time region (E/LTR). It was observed that the ETR permeability is less sensitive to pore pressure compared to the LTR permeability. Moreover, it was observed that the LTR permeability continuously increase with the reduction of pore pressure from 4500 psi to 250 psi, while for ETR there is no consistent change in measured permeability. As it was expected, with an increase in net stress, both ETR and LTR reduced dramatically.

We apply our methodology to simultaneously model the gas flow in shale samples and to present an equation by which gas permeability can be predicted for any pore pressure and net stress.

The results of this study, can be used to generate more reliable simulation models of shale reservoirs with focus on the UK based formations. Invaluable experimental data presented in this study are also helpful for exploiting shale reservoirs in the UK both for clean energy production and gas storage purposes.

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MS06-B / 941

Irreversible processes, inertial effects, and collective filling in geometries of increasing complexity

Author: Ivan Lunati[1]

Co-author: Andrea Ferrari [2]

[1] *Empa*

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Today experimental and computational resources allow visualizing transport phenomena in idealized or more realistic pore geometries and modeling these processes starting from the first principles of continuum mechanics (i.e., solving momentum- and mass-conservation equations by means of tools borrowed from classic Computational Fluid Dynamics).
We briefly introduce these computational methods, which have become increasingly popular over the last decade, and focus on the Volume Of Fluid method, which has been validated against multiphase-flow experiment in pseudo two dimensional porous media 1 and has been used to elucidate the relationship between capillary pressure and the total surface energy of the system [2].
Then, we investigate the role of local inertial effects in influencing the morphology of the invading front [3]. We pay particular attention to the characterization of abrupt events, to collective pore filling, and to the effects of geometries of increasing complexity [4]. We discuss how local inertial effects, resulting from surface energy instabilities and subsequent spontaneous reconfiguration of the interface, cannot be avoided and how these processes are at the basis of hysteresis.

Participation:

In-Person

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Energy Transition Focused Abstracts:

942

A Systematic CO2 Huff-n-Puff Injection Approach for Enhanced Condensate recovery and CO2 storage.

Authors: Ifeanyi Seteyeobot[1]; Mahmoud Jamiolahmady[2]

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This paper presents an experimental and simulation study to adequately identify the level of CO2-Gas Condensate (CO2-GC) interaction during CO2 Huff-n-Puff injection in depleted gas condensate reservoirs for enhanced condensate recovery (ECR) and CO2 storage. In this study, appropriate experimental phase behavior analysis and Equation of State (EOS) modeling were conducted using synthetic-rich gas condensate mixtures. The results highlight the importance of EOS tuning in compositional modeling, especially as the fluid composition varies significantly in the reservoir and in cases where the injected fluid is different from the resident fluid, particularly when the injected fluid is CO2. A total of four injection cycles with incremental CO2 volumes relative to the initial resident fluid volume prior to expansion were considered.

The observed PVT data was applied in designing a systematic CO2 Huff-n-Puff injection technique considering the level of interaction between CO2 and resident fluid at the maximum condensate saturation of the corresponding CO2-GC fluid mixture. This technique differs from the conventional CO2 Huff-n-Puff injection method as it successfully optimizes the CO2 injection pressure and volume.

Experimental results revealed that condensate recovery would be enhanced similar to the conventional CO2-Huff-n-Puff approach but with the added benefit of lower volumes of CO2 injected and produced. The experimental results suggest condensate swelling and revaporization as the dominant recovery mechanisms when the proposed CO2 H-n-P injection technique was implemented. The recovery potential of the proposed method is further investigated on different rock samples, including high, low, and ultra-low permeability cores. Results suggest that although the proposed condensate treatment technique can significantly alleviate condensate banking problems in Ultra-low and low permeability gas condensate reservoirs, the condensate recovery and CO2 storage efficiency are more profitable when implemented on high permeable reservoirs.

Participation:

Online

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Poster / 943

Pore Scale Modeling of roots and soil interaction

Authors: Maximilian Rötzer[1]; Alexander Prechtel[2]; Nadja Ray[1]

[1] *Friedrich-Alexander Universität Erlangen-Nürnberg*

[2] *Mathematics Department, University of Erlangen-Nürnberg*

Corresponding Authors: nadja.ray@ku.de, maximilian.roetzer@fau.de, prechtel@math.fau.de

We present a spatially and temporaly explicit mathematical model for root-soil interaction at the microscale. This includes a cellular automaton model for dynamic rearrangement of soil particles combined with a particulate organic matter turnover model. Additionally, the impact of root growth and root exudates and their distribution into the soil on soil aggregation and stability are taken into account.

We address the questions how soil aggregation and a growing root mutually interact in soils of different texture. We quantify how root shapes the rhizosphere and the bulk for instance by evaluating the respective dynamical change in porosity.

Participation:

In-Person

References:

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Poster / 944

High-resolution Darcy-Brinkman simulation of wormhole growth based on X-CT data.

Authors: Michał Dzikowski[1]; Rishabh P. Sharma[2]; Piotr Szymczak[1]

[1] *Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland*

[2] *Faculty of Physics, University of Warsaw, Poland*

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In 2022 a number of pre-exascale and exascale supercomputers had become available for scientists. We took the opportunity of the pilot phase of the LUMI supercomputer to perform a number of simulations of wormhole growth with an aim to use as much spatial information as possible. The goal was to investigate if properties of growing wormholes could be recovered if sufficient resolution is assured, and how porous matrix-wormhole interaction changes with CT resolution. Additionally, samples used in this study underwent experimental studies. They were scanned before and after the experiment, as well as during the dissolution. This 4D tomographic data and pressure history provided necessary input for high-res simulations as well as validation framework.

As the LUMI computer, as well as most of the newly built HPC machines, is based on GPUs we decided to use the Lattice Boltzmann code as main flow and transport solver. LBM has significant number-crunching performance thanks to its intrinsic parallelization properties which was paramount for this study. Based on an open-source, highly parallel multi-GPU TCLB solver, we design the model capable of handling Darcy - scale simulations with the initial porosity fields constructed based on X-ray microtomography images. In particular, we analyze the reactive-infiltration instabilities, which lead to the formation of dissolution fingers (wormholes), in which both the flow and reactant transport become spontaneously localized. Since dissolution fingers dramatically increase permeability of the rock, wormholing is important both for industrial applications and in hydrogeological studies. The main problem in modeling of wormholing is a multi-scale character of this process, with flow and transport near a wormhole tip strongly coupled to the macroscopic geometry of the emerging structures. The ability to perform large scale parametric and sensitivity studies of wormholing constitutes thus an important addition to experimental studies, hence the need for a high throughput simulator.

We test our numerical predictions against the data from time-lapse dissolution experiments in an aim of constructing a predictive model capable of recovering time evolution of 3D wormhole shape based on the initial X-ray tomography data.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS02 / **945**

S table water isotopologue fra ctionation during soil water evaporation: Analysis using a coupled soil atmosphere model

Authors: Stefanie Kiemle[None]; Katharina Heck[1]; Edward Coltman[2]; Rainer Helmig[3]

[1] *University Stuttgart*

[2] *University of Stuttgart IWS-LH2*

[3] *University of Stuttgart*

Corresponding Authors: edward.coltman@iws.uni-stuttgart.de, rainer.helmig@iws.uni-stuttgart.de, katharina.heck@iws.uni-stuttgart.de, stefanie.kiemle@iws.uni-stuttgart.de

The atmosphere-soil system forms a highly coupled system, which makes key processes such as evaporation complex to analyse as the mass, energy and momentum transfer is influenced by both domains. To enhance the understanding of evaporation processes from soils, stable water isotopologues are suitable tools to trace water movement within these systems as heavier isotopologues enrich in the residual liquid phase. Due to the complex coupled processes involved in simulating soil-water evaporation accurately, quantifying fractionation during flow and transport processes at the soil-atmosphere interface remains an open research area. In this work, we present a multi-phase multi-component transport model that resolves flow through the near surface atmosphere and the soil, and models transport and fractionation of the stable water isotopologues using the numerical simulation environment DuMuX. Using this coupled model, we simulate transport and fractionation processes of stable water isotopologues in soils and the atmosphere by solving compositional flow equations and by using suitable coupling conditions at the soil-atmosphere interface instead of commonly used parameterization.

In a series of examples of evaporation from bare soil, the transport and distribution of stable water isotopologues are evaluated numerically with varied conditions and assumptions, including different atmospheric conditions (turbulent/laminar flow, wind speed) and their impact on the spatial and temporal distribution of the isotopic composition. Building on these results, we observed how the enrichment of the isotopologues in soil is linked with the different stages of the evaporation process. A qualitative study is conducted to verify single fractionation processes in our approach. As an outlook, we will present how the coupling of the free-flow and the porous medium domain allows us to use atmospheric measurements (which are often conducted at 2 m above the soil surface) and account for convective transport in the free-flow region. Thus, we can validate our results by using field-scale lysimeter experiments.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / 946

Time-lapse imaging of fine particle movement in porous materials

Authors: CHENZI SHI[None]; LIN MA[None]; KEVIN TAYLOR[None]

Corresponding Authors: lin.ma@manchester.ac.uk, chenzi.shi@postgrad.manchester.ac.uk, kevin.taylor@manchester.ac.uk

Particulate flow in porous materials is a common phenomenon and also one of the big challenges in flow dynamics. As one example, fines migration within porous rocks may block the pores and reduce the permeability, leading to formation damage in subsurface reservoirs. Varied physical and chemical parameters causing fines migration have been widely studied in many subsurface applications such as geothermal exploitation, oil and gas extraction and carbon storage. However, the directly

imaged evidence of porous structure changes and formation damage is still limited, which makes the theoretical understanding of particulate flow challenging. This research has applied a combination of two-dimension (2D) in-situ time-lapse radiography and three-dimension (3D) X-ray tomography imaging techniques under in-situ sample environment to directly image and characterise the fines migration and deposition in porous materials.

Time-lapse imaging experiment was performed at a high flux X-ray tomography scanner at National X-ray Computed Tomography facility with within an in-house designed and 3D printed high-pressure flow cell. A course-porous (pore size around 80-120 μm) and a fine-porous (pore sizes around 40 μm) sandstones and mix-size sintered glass beads (half pores around 80-120μm and half pores <50μm) to form porous bed to analogue three different porous structure systems. A suspension fluid contains calcium carbonate powder (12μm) flew through the porous bed and deposited inside and on top of the porous samples and this progress was captured using time-lapse radiography images. X-ray tomography was performed before and after the experiment to quantify the pore structure change and the deposition of particles. The results show that fine particles tended to fill the pores evenly in the well-connected pore structure with larger pores (around 40-60μm) transformed to small pores(20-40μm). Both internal and external filter cake were formed. While in the poorly connected porous structure, pores filled the preferred flow pathways first and formed the external filter cake. This imaging experiment quantified the fines migration deposition and migration within the porous materials and the effects of pore structure controls spatially and temporally. The results have improved the theoretical understanding of fine particles migration and deposition within varied porous structure and will have wide applications in subsurface engineering, materials sciences and material engineering.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

947

Bulk and leading-edge dynamics in glioblastoma invasion

Author: Dumitru Trucu[1]

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Abstract:
Despite significant recent advancements, the complex multi-scale brain tumour invasion patterns in 3D are still poorly understood. A particular role in the invasion patterns of the collective migration of the glioblastoma cells populations is likely played by the distribution of micro-fibres, and to address this aspect, in this talk we present our recent advances in this direction. Specifically, we will focus on our recent 3D multiscale mathematical modelling and computational development that builds on our previously introduced 2D multiscale moving-boundary framework and that is able to address the 3D multiscale tumour dynamics. T1 weighted and DTI scans are used as initial conditions for our model, and to parametrise the diffusion tensor. Numerical results show that including an anisotropic

diffusion term may lead in some cases (for specific micro-fibre distributions) to significant changes in tumour morphology, while in other cases, it has no effect. This may be caused by the underlying brain structure and its microscopic fibre representation, which seems to influence cancer-invasion patterns through the underlying cell-adhesion process that overshadows the diffusion process.

Participation:

Online

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Energy Transition Focused Abstracts:

948

Porous design of the nasal ducts of Arctic animals for efficient air heating and moistening: An entropy generation approach

Authors: Natalya Kizilova[1]; Signe Kjelstrup[2]; Hyejeong Cheon[3]; Øivind Wilhelmsen[4]; eirik flekkøy[5]

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[2] *Norwegian University of Science and Technology, NTNU, Trondheim*

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[4] *PoreLab, Department of Chemistry*

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Sophisticated porous structures are commonly used in nature for efficient heating/cooling, mixing, uniform distribution of fluids and their components. Arctic animals have gained very efficient heating systems in their nasal ducts 1 and their design can be used for optimization of chemical reactors [2], heaters/coolers and other engineered units. Among them are spiral-type 1, fractal-type [3], and porous-type structures in the nasal ducts of Antarctic, desert and other animals accommodated to extremal ambient conditions. Thermodynamic approach can be helpful in (i) understanding the physical mechanisms underlying the porous structure and function of the tissue/organ; (ii) understanding the evolutional optimization processes; (iii) reasonable implementation of the nature-inspired design in engineered systems. The shape optimization approach based on minimal viscous or thermal dissipation is widely used in mechanical, chemical, biomedical and aerospace engineering, while the minimal entropy generation Sirr approach combines both of them as well as other dissipation sources in one optimization criteria Sirr⊠min.

Here the porous design of the nasal ducts of seals and its efficiency for heating/moistening the inhaled cold dry air and cooling/drying the exhaled air is studied based on non-equilibrium thermodynamics. Detailed geometry of the structure was determined from CT images. The volume of the air passages along the duct Va(z) determines the hydraulic resistance for the flow, while the surface area Sa(z) of the porous structure that is is direct contact with air provides the heat conduction and water evaporation/absorption.

An equivalent 1D model of the nasal duct as a tube with the same functions Va(z) and Sa(z) is considered. The governing equations for the temperatures and water concentration in the air and several tissue compartments (mucus, interstitia, arteries and veins) have been obtained from general heat

and mass balance equations. The cross-coupled heat and mass transfer phenomena are taken into account. Solution of the system has been composed for different boundary conditions and model parameters by numerical methods. The mean axial velocity, pressure, temperature and water vapor concentrations in each cross-section of the porous structure have been computed as functions of the longitudinal coordinate. The entropy production Sirr due to the irreversible physical phenomena in the system has been computed as a function Sirr(z) along the duct.
It was shown that the complexity of porous structures in the nasal cavity of Arctic seals ensure their high efficiency for the heating/moistening of the inhaled air at low ambient temperatures till -30C compared to the Mediterranean seals which can hardly survive in such low temperatures. The importance of the surface/volume ratio Sa/Va(z) for the heating/cooling and moistening/drying of the air or gas flow has been studied. It is shown the entropy production Sirr is an important parameter for the shape optimization of the fluid-flow based systems. The input of the heat dissipation, pressure loss and viscous dissipation to Sirr is revealed. The contributions to the energy dissipation from heat flow, viscous flow and moisture loss is discussed. Possible engineered applications of the nature inspired porous structures are listed. An importance of minimum entropy generation principle is discussed.

Participation:

Online

References:

1 Solberg S.B.B., Kjelstrup S., Magnanelli E., Kizilova N., Barroso I.L.C., Acquarone M., Folkow L. (2020) Energy-Efficiency of Respiration in Mature and Newborn Reindeer. J. Compar. Physiol. B, 190, 509-520. doi: 10.1007/s00360-020-01284-3
[2] Magnanelli E, Solberg SBB, Kjelstrup S (2019) Nature-inspired geometrical design of a chemical reactor. CHERD 152:20–29. doi: 10.1016/j.cherd.2019.09.022
[3] Sauermoser M., Kizilova N., Pollet B.G., Kjelstrup S. Flow Field Patterns for Proton Exchange Membrane Fuel Cells. // Front. Energy Res. –2020. –v.8, 13. doi: 10.3389/fenrg.2020.00013

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Energy Transition Focused Abstracts:

MS06-A / **949**

Pseudo-Thermodynamics of Immiscible Two-Phase Flow in Porous Media: Differential Geometry and Convenient Coordinates

Author: Håkon Pedersen[1]

Co-author: Alex Hansen [1]

[1] *NTNU*

Corresponding Authors: alex.hansen@ntnu.no, hakon.pedersen@ntnu.no

The problem of immiscible and incompressible two-phase flow in porous media can be recast in terms of the average seepage velocity of the wetting- and non-wetting fluids and a novel velocity called the co-moving velocity, which has the potential of simplifying the theoretical description of macroscopic flow properties 1. The theory is based on degree-1 Euler homogeneity of the total volumetric flow rate through the porous medium, and the framework takes on the appearance of a thermodynamic

theory. The co-moving velocity is the quantity that bridges the gap between the measurable seepage velocities and the abstract thermodynamic velocities that appear in the thermodynamic theory. It has been shown both numerically and experimentally that the co-moving velocity has a particularily simple behaviour [2], and understanding the role of this quantity in a more general theoretic setting might aid our intuition for this abstract velocity.

We will present different interpretations of the transformation from the seepage velocities to the total seepage- and co-moving velocity in the context of a pseudo-thermodynamic theory with as few variables as possible. This will lead us to make the connection between the flow quantities and differential geometry, and show that one is able to regain results from previous works and uncover new descriptions of the flow by convenient coordinate-changes on the space of extensive pore-areas. We discuss a general description of the flow-quantities based on vector fields, and the relation between our framework and the broader field of geometric thermodynamics.

Participation:

In-Person

References:

1 Hansen, A., Sinha, S., Bedeaux, D., Kjelstrup, S., Gjennestad, M. A., & Vassvik, M. (2018). Relations Between Seepage Velocities in Immiscible, Incompressible Two-Phase Flow in Porous Media. Transport in Porous Media, 125(3), 565–587. http://dx.doi.org/10.1007/s11242-018-1139-6

[2] Roy, S., Pedersen, H., Sinha, S., Hansen, A. The Co-Moving Velocity in Immiscible Two-Phase Flow in Porous Media. Transp Porous Med 143, 69–102 (2022). https://doi.org/10.1007/s11242-022-01783-7

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Energy Transition Focused Abstracts:

MS08 / 951

Quantification of Coupled Longitudinal and Transverse Dispersion in Porous Media

Authors: Lesley James[1]; Saied Eskandari[None]

[1] *Memorial University of Newfoundland*

Corresponding Authors: se2284@mun.ca, ljames@mun.ca

This study uses an experimental approach to estimate the average longitudinal and transverse dispersion coefficients in a homogeneous, non-uniform, and anisotropic porous medium during miscible displacement. Traditionally, most miscible displacement studies have focused on recovery factor and recovery mechanism and the Peclet number is used to find the dispersion and diffusion coefficients from mathematical correlations. This study employs a unique method to estimate the longitudinal and transverse dispersion coefficients. A unique image processing tool is developed and used to analyze the developing mixing zone. Concentration profiles from the processed images are then used to collaborate with Bayesian estimator tool, which is developed to find the dispersion coefficients in the analytical solution of the Convection-Diffusion Equation (CDE). The results confirm that both longitudinal and transverse dispersion coefficients strongly depend on

the velocity of the displacing fluid. The effects of anisotropy on miscible mass transport are investigated in this study using this unique method and longitudinal and transverse dispersion coefficients are estimated.

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A Microfluidic Platform to Study Asphaltene Deposition; Studying the Effect of Operating Conditions

Authors: Sepideh Alimohammadi[1]; Juan Esteban Jaramillo Velez[None]; Maziyar Mahmoodi[2]; Lesley James[1]

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Asphaltenes are analogous to the "cholesterol"of crude oils, so they may cause significant flow assurance problems to various oil and gas processes such as the plugging of pipelines, the damage of rock formations, and the stabilization of viscous water-in-oil emulsions, and negatively affect the economy of the oil recovery, transportation, and processing by increasing operational expenditures (OPEX). Having a comprehensive understanding of the interfacial behaviour of asphaltene helps researchers to accurately design solutions for the asphaltene related issues. In this work, the microfluidic devices and image analysis is used to visualize fluid flow in porous media and investigate asphaltene deposition. Effect of operating conditions on asphaltene deposition is important, however, it has been investigated in very few research works. This study examines the effect of operating conditions, e.g., pressure and gas injection, on asphaltene deposition in the porous media using microfluidic platform. Conducting experiments under different operating conditions alters the amount of asphaltene deposition due to changes in the amount of asphaltene precipitation (changing the solubility of asphaltene in oil mixture) and deposition mechanisms, e.g., adsorption. To capture these phenomena, an automated image-based computational technique was used to assess high-fidelity information on asphaltene deposition in a microfluidic device. For this purpose, the advanced image-processing algorithm was used in LabVIEW to evaluate the quantity of asphaltene deposition. The asphaltene was extracted from Athabasca oil with the initial content of 15 wt%. A method by combining ASTM D2007-80 and ASTM D6560-00 was used to double wash asphaltene by toluene and using a Soxhlet. Then, the synthetic oil was made with the same asphaltene content of the original oil of 85 wt% toluene and 15 wt% dried asphaltene. The deposition of asphaltene was visualized using a high-resolution camera (Canon 6D) and a 105 mm macro lens. The image processing technique is able to accurately measure the quantity of deposition within the micromodel using different operating conditions. The research also suggested that microfluid devices offer a reliable and unique reproduction of porous media that can be used to study the flow assurance issues.

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Energy Transition Focused Abstracts:

MS14 / 954

Multiphase Flow Effects on a Physics-Based Shale Reservoir Production Forecasting Model: A Global Sensitivity Analysis

Authors: Daniela Arias Ortiz[None]; Tadeusz Patzek[1]

[1] *King Abdullah University of Science*

Corresponding Authors: tadeusz.patzek@kaust.edu.sa, danielaandrea.ariasortiz@kaust.edu.sa

The generalized physics-based scaling curve method proposed by Patzek et al. (2013) is an excellent alternative to the decline curve methods that forecast gas production from shale reservoirs. However, it still neglects the multiphase flow effects and may lead to unreliable hydrocarbon production prediction from mudrock reservoirs. In this study, we perform a global sensitivity analysis using a compositional reservoir simulator to analyze the sensitivity of the scaling factors describing the physics-based method to multiphase flow effects varying selected input factors. We built a conceptual reservoir model of a typical, hydraulically fractured shale condensate gas well using a commercial reservoir simulator. We select the fluid input factors and their range of possible values over which we analyze the scaling curve. We perform a space-filling design using the MaxiMin Latin Hypercube sampling method. We run our simulation tests and estimate the scaling parameters: characteristic time of pressure interference between neighboring hydraulic fractures (τ) and hydrocarbon mass in place in the stimulated reservoir volume ($\mathcal{M}_{SRV}$). We then calibrate a surrogate model to map the relationship between the multiphase flow properties and the scaling parameters using Bayesian optimization. Finally, we identify the key parameters affecting the shale condensate gas mudrock plays forecasting using global sensitivity analysis ("Sobol" indices). Our results show the relative contribution of the multiphase flow input factors of the reservoir simulator to the variance of the physics-based curve scaling parameters. We demonstrate the importance of reservoir permeability, initial condensate/gas ratio (CGR), initial reservoir pressure, wet-gas phase behavior, and hydraulic fracture spacing in the variations of $\mathcal{M}$ and τ. We show that the mudrock ultimate recovery factor (EUR) prediction when the condensate saturation around the wellbore is below a critical saturation may be accurately estimated using the single-phase solution. Finally, we highlight the limitations of using the single-phase physics-based scaling curve method to forecast condensate gas production from low-permeability reservoirs.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS01 / **957**

Visualizing the Effect of Gravity on Hydrogen Redistribution at Pore Scale

Author: Omid Shahrokhi[1]

Co-authors: Amir Jahanbakhsh [1]; Puyan Bakhshi [1]; John Andresen [1]; M. Mercedes Maroto-Valer [1]

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Hydrogen is considered a low-carbon fuel that can potentially contribute to the large-scale decarbonization of different sectors, including power generation, heating, transportation, and industry. Blending hydrogen into national gas distribution networks can also help decarbonize distributed carbon emissions from domestic consumers where carbon capture is not feasible. More pilot projects worldwide, such as H100 Fife and HYDeploy2 in the UK and HyGrid in Long Island, US [1–3], are showcasing the use of hydrogen in the national gas networks. The reliable and robust operation of a gas network at the national scale (12 to 51TWh of hydrogen in the case of the UK national gas network [4]) would critically require safe and efficient large-scale hydrogen storage. As an example, to meet the UK's seasonal demand and production variations from intermittent renewable energies, 0.37-1.58 billion cubic meters of hydrogen storage capacity is required which represents 25-105% of the current UK strategic natural gas storage capacity [5]. This means large-scale repurposing of current storage sites (both salt caverns and depleted gas reservoirs) and the development of new sites. To unlock the large-scale storage capacity of depleted gas reservoirs and saline aquifers for efficient hydrogen storage, understanding the flow and trapping mechanisms of hydrogen at the pore scale in contact with resident fluids is essential. To achieve this, a set of experiments is designed to explore the fluid distribution in cyclic fluid displacements representative of seasonal storage and production of hydrogen in subsurface reservoirs. These cyclic flow experiments are performed in a sandstone core and the fluid distribution at the pore scale is imaged by an X-ray micro-computed tomography (micro-CT) rig with a cubic voxel size of 3x3x3 microns. To achieve the highest imaging resolution with our in-house testing rig, a core sample size of 5mm diameter and 10mm length is selected. The outlet pressure is maintained by the receiving pump at 7.0 MPa. The fluids are injected through the core at a constant flow rate of 5 mL/hr to ensure capillary-dominated flow. Potassium iodide (KI) salt is dissolved as a dopant in the brine to provide effective contrast between the brine, hydrogen, and rock sections of the images. To ensure gravity-stable fronts, hydrogen is injected from the top and brine from the bottom of the core holder. The alternate injection of hydrogen and brine is then performed until no significant change in saturations is observed along the sample. After gas injection an average hydrogen saturation of 32% is observed in the core sample, however, about 6% fluctuation in saturations is observed. The core is then isolated for 30 days, and the imaging experiment was repeated. The amount of the displaced hydrogen by buoyancy effect and its distributions is then discussed. This provides insight into hydrogen displacement by gravity forces. Ongoing studies are investigating the trapping of hydrogen at similar flow conditions at the pore and core scale.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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MS06-A / **959**

Dissolution of trapped CO2 in carbonates rock at high pressure and high temperature conditions using X-ray micro-tomography

Author: Abdul Hakim Mazeli[None]

Co-authors: Hannah Menke [1]; Julien Maes [1]; Kamaljit Singh [1]

[1] *Heriot-Watt University*

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Capillary trapping is an effective and rapid mechanism for CO2 storage in underground formation, which has been studied by many researchers. However, the long-term storage of trapped CO2 can be affected due to its dissolution into non-CO2 equilibrated brine. Understanding the mass transfer of CO2 into formation brine both qualitatively and quantitively is crucial for improving the security of geologic carbon storage. The aim of this project is to develop an understanding of the trapped CO2 dissolution behavior in carbonate rocks using X-ray micro-tomography. In this project, CO2-brine flow experiments were performed using a unique X-ray transparent flow apparatus, specifically designed for 120 ℃ and 200 bar. After establishing the residual saturation of supercritical CO2 (i.e., trapped CO2) using CO2-equilibrated brine, the sample was scanned after injecting pre-determined pore volumes (e.g., 0.5 PV, 1.0 PV) of non-CO2 equilibrated brine. The results shows that CO2 saturation decreases from 17.34% to 7.5% with 1 PV injection of non-CO2 equilibrated brine. In spite of slow injection rate, two unique pore-scale processes were observed, i.e., CO2 dissolution and CO2 re-mobilisation. This study will be extended to 4D (i.e., time-resolved 3D) synchrotron imaging to obtain a better understanding of these interlinked dynamics.

Participation:

In-Person

References:

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Poster / 960

Polymer Thermal Degradation: Numerical Simulation and Upscaling for Field Scale Reservoir Applications

Author: Abdulaziz Alsaleh[None]

Co-authors: Martin Blunt [1]; Ann Muggeridge [1]

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Thermal degradation is a key element that determines the success of polymer projects. The published work conducted on commercial polymers such as HPAM has suggested the infeasibility of polymers used in harsh reservoir environments. Nonetheless, with recent advances in polymer technology interest in numerical simulation evaluation on field-scale harsh reservoir environments has revived. In this project, we aim to study the impact of thermal degradation, hydrolysis reaction, and salinity simultaneously on polymer flood performance in a full field scale heterogeneous and harsh reservoir environment. A set of sensitivities on operating parameters will set the strategy to minimize the impact of degradation of polymer flood performance. To reduce the computation time of full-field scale numerical simulation a workflow and method to upscale the polymer degradation model will be established to facilitate an efficient simulation computing time.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

961

Spatial permeability evaluation in carbonate rocks using spin echo magnetic resonance imaging at 0.6 T

Author: Adam Fheed[1]

Co-author: Artur Krzyżak [1]

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Intensive diagenesis and unprecedented contribution of organisms are often reflected in complex internal structure of carbonate rocks. The related values of permeability coefficient may thus show observable changes even at plug scale. The majority of existing permeability estimation workflows either only deliver a whole-sample value of this parameter or its distribution in one direction. Considering high complexity of carbonates, this study aims to develop a new way of slice-to-slice permeability estimation in at least three directions using nuclear magnetic resonance imaging. The model is based on a modified form of the SDR equation, where transverse relaxation time log mean (T2lm) is computed for a number of slices acquired within a small plug sample. Two plugs representing reef carbonates of the Late Permian Zechstein Limestone formation (Ca1) of West Poland were tested. Their diameter and height were roughly 2.54 cm and 1.2 cm, respectively. Whole-sample and slice measurements were performed on plugs saturated with demineralized water. Eight images representing 1.5 mm-thick slices were acquired and stacked for each plug under different echo time values using Spin-Echo 2D sequence at 0.6 T. The echo times used for slices were: 7, 14, 28, 42, 56, 70 and 84 ms, whereas the corresponding echo time range for whole-sample scans was from 7 to 327 ms. The repetition time was equal to 3000 ms, number of scans was 32 and the resolution of the images was 0.5 mm × 0.5 mm × 1.5 mm. MATLAB software was used to compute the whole-sample T2lm by bi-exponential curve fitting to signal intensity vs. echo time data. Mercury Injection Capillary Pressure (MICP) measurements were carried out to obtain global plug permeability, while low-field NMR relaxometry studies of saturated samples gave global porosity. The low-field experiments were realized at 0.05 T using echo time of 100 μs and number of scans equal to 256. The whole-sample T2lm, global MICP permeability, and low-field NMR porosity were used to compute the calibration factor in the SDR equation. Having resolved the factor and derived slice-to-slice porosity by calibrating the MRI data to the global porosity value, slice permeability in xy, xz and yz planes was estimated. Lastly, pore geometry was verified using transmitted light polarizing microscopy. The obtained results delineated different sample characteristics with permeability ranging from several to several tens of mD. The porosity-permeability relations were also variable, giving the determination coefficients of 0.57 and 0.94 for samples characterized by average permeability close to 7 mD and 40 mD, respectively. Such results were compliant with pore geometry observed at microscopic scale, where worse permeability could be attributed to less uniform pore size distribution and weaker pore communication. It seems that the proposed workflow can help determine the causes of small-scale permeability changes as well as identify the potential risks of abrupt permeability reduction in chosen reservoir regions. Complex reservoir characterization would, however, require extending the population of samples.

Participation:

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References:

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Energy Transition Focused Abstracts:

MS15 / **962**

Accelerating continental-scale groundwater simulation with a fusion of machine learning, integrated hydrologic models and community platforms

Authors: Reed Maxwell[1]; Laura Condon[2]

Co-authors: Elena Leonarduzzi [1]; Yueling Ma [1]; Andrew Bennett [2]; Hoang Tran [3]; Peter Melchior [1]

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Today, water and resource managers face a huge challenge managing systems that are rapidly evolving in a warming climate, and where historical observations are no longer a reliable guide. Existing water management tools significantly lag the state of the science and are often ill-equipped to provide reliable forecasts under these conditions. Similarly, historical observations are of limited use on their own, without additional modeling and analysis. Simulations with integrated hydrology models (that solve the 3D Richards' equation and 2D shallow water equations in a globally-implicit manner) provide robust results all the way to continental scales, yet are computationally expensive, running on supercomputers. Our approach trains Machine Learning (ML) emulators of integrated hydrology models to drastically reduce the computational burden. We combine these emulator approaches with both purely data-driven approaches and Simulation-Based Inference, to generate seasonal to annual hydrologic scenarios of both groundwater and surface water systems using observations and sophisticated physics-based hydrologic models. This talk will highlight the technical challenges of this rapidly developing branch of hydrologic modeling and discuss the platform we have developed, HydroGEN, which provides seasonal forecasts over the Continental US (CONUS). We will also the path forward for this platform and ongoing work to develop inclusive and diverse pilot studies.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

963

Corner flow Impact in forced imbibition by color lattice Boltzmann model

Authors: Jianchao Cai[1]; Yang Liu[None]; Steffen Berg[2]; Yang Ju[3]

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Capillarity in porous media plays a crucial role in many engineering and industrial processes, such as enhanced oil recovery and groundwater contamination remediation. Due to the instabilities at the two-phase interface, the defending fluids in these processes are often not effectively displaced. Therefore, it is of great significance to study capillary-driven flow in natural rocks at the pore scale, especially under the completely wetting and viscously unfavorable conditions due to their contribution to interfacial instability. In this work, numerical simulations of forced imbibition in three natural porous media are carried out at four different injection rates based on the color lattice Boltzmann model. The interfacial evolution and in situ fluid distribution are analyzed from several perspectives. Results show that as the capillary number, expressed in logarithms, varies from −2.5 to −4.0, the flow characteristics of the invading fluid change from leading films on the solid surface of large pores to corner flow along the pore corners of pores with different sizes, the dominant pore filling event changes from ganglion dynamics to snap-off trapping, and the morphology of the displacement front changes from viscous fingering to a rough but uniform characteristic. These changes at the two-phase interface determine the fluid distribution and fluid structure, controlling the microscopic displacement efficiency, interface area and fluid connectivity. This work investigates for imbibition of the local and global flow physics and dynamics, the mechanical nature and the resulting effects of interfacial instability under unfavorable conditions, which help to deepen our understanding of the microscopic mechanism of forced imbibition.

Participation:

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Energy Transition Focused Abstracts:

967

Electrolyte Wetting in the Production of Lithium-Ion Batteries: A Simulation Approach on Multiple Scales

Author: Stefan Rief[1]

Co-authors: Konrad Steiner [1]; Dariusz Niedziela [1]; Jochen Zausch [1]; Stephan Hoecker [1]

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Driven by electromobility, the demand for lithium-ion batteries is strongly rising. Hence, it is imperative to increase the production capacities by optimizing production processes. After cell assembly, an important but time-consuming step is the addition of the liquid electrolyte. It is supposed to fill the electrode and separator pores homogenously. Driven by capillary forces and external pressure, the wetting process may take several hours. Moreover, since there is no inline characterization of the wetting state yet, duration and process control are often based on experience or trial and error.
We propose to support process design by numerical simulations on multiple scales: On the macroscopic cell scale, we developed a new approach based on extended Navier-Stokes-Brinkman equations considering capillary forces as major driving force. Furthermore, the model does not only account for the effective electrolyte flow, but also for the residual gas-phase inside the pores. The new approach was implemented in our software framework CoRheoS FLUID enabling the computation of time and space evolution of the electrolyte distribution.
As input parameters, the outlined cell-scale approach requires knowledge of the saturation dependent capillary pressure and the permeability of the microstructures present in the sheet stack of the cell, i.e. anode, separator and cathode. To obtain those quantities, we perform microstructure simulations of fully resolved representative parts of the sheets. For structure generation and property computation, the software GeoDict is used.
In this presentation, we will describe our models and workflow starting from the relevant microstructure analysis with GeoDict and the subsequent macroscale, time-dependent wetting simulation with CoRheoS FLUID.

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Poster / 968

Flow, heat, and transport at the scale of grains and pores in porous building materials

Authors: Hannah Menke[1]; Julien Maes[1]; Kamaljit Singh[1]

[1] *Heriot-Watt University*

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The transport of moisture and heat through building materials ultimately dictates their insulation performance over its lifetime. However, characterisation of building materials is challenging because porous building materials are heterogeneous and their macroscopic physical properties (e.g. permeability, thermal, and mechanical) depend on their micro scale characteristics, i.e. the local

distribution and features of the solid components and the connectivity of the spaces between them. Large-scale testing can measure these macro-scale properties, but often does not give insight into the underlying structural properties that ultimately leads to optimisation. Thus, a knowledge of the 3D structure is therefore required to assist in the development and implementation process. Experiments combining X-ray microtomography with numerical modelling are an accepted method of studying pore scale processes and have been used extensively in the oil and gas industry to study highly complex reservoir rocks. However, despite the obvious similarities in structure and application, these techniques have not yet been widely adopted by the building and construction industry.

We have experimentally investigated the pore structure of several building materials using X-ray tomography and direct numerical simulation. Four samples were imaged at between a 6 and 15 micron resolution inside a micro-CT scanner. The porosity and connectivity were extracted with the grain, throat, and pore size distributions using image analysis. The permeability, moisture transport, and heat flow were then solved using GeoChemFoam, our highly versatile and open-source numerical solver. The heat and transport were then upscaled to create a custom heat and transport dispersivity for each material. This is the first multi-scale study of structure, flow and transport on building materials and this workflow could easily be adapted to understand and improve designs in other industries that use porous materials such as fuel cells and batteries technology, lightweight materials and insulation, and semiconductors.

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In-Person

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Poster / 969

Advanced mesoporous thin film characterisation by ellipsometric porosimetry

Author: Mate Furedi[1]

Co-authors: Bálint Fodor [2]; András Marton [2]; Alberto Alvarez-Fernandez [3]; Péter Basa [2]; Stefan Guldin [1]

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Mesoporous architectures in thin film configurations (< 10 μm) are promising class of materials for a range of applications, including antireflective coatings 1, electrochemical sensors [2], and electrode materials [3] among others. The low quantity of solid contained in such thin films makes

their structural characterisation with conventional methods developed for bulk materials (e.g. N2 porosimetry) challenging [4]. Ellipsometric porosimetry (EP) is an alternative, purely optical characterisation technique based on spectroscopic ellipsometry, enabling the study of very thin, porous layers in a non-destructive way through acquiring refractive index, extinction coefficient and thickness information based on the change of polarization of the reflected light. Ellipsometric spectra are acquired at different relative pressures of a gas phase adsorptive to construct a volume adsorbed isotherm via effective medium approximations. Since the characterisation is purely optical without requirement for volumetric or gravimetric information of the adsorptive, the accuracy of measurement is independent of the quantity of the studied adsorbent film, hence reliable information can be obtained for limited sample sizes (in terms of thickness and lateral extension).

In this work, the mesoscale characterisation of porosity, pore size distribution and specific surface area via EP is presented, as well as advanced methods for the investigation of mechanical strength (Young-modulus) [5] and microscopic wettability [6]. A wide range of porous architectures and surface chemistries were explored to provide guidance on the technique's applicability with suitable adsorptives, such as water, toluene, methanol, and other organic liquids.

Participation:

In-Person

References:

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https://doi.org/10.1016/j.tsf.2023.139683.

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Energy Transition Focused Abstracts:

973

Evolution of porous rock permeability under cyclic confining pressure

Author: Evgenii Kozhevnikov[1]

Co-authors: Mikhail Turbakov [1]; Evgenii Riabokon [1]; Evgenii Gladkikh [1]; Vladimir Poplygin [1]; Mikhail Kriukovskii [1]

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An increase in effective pressure causes deformation and a decrease in the conductivity of natural porous media - rocks. Also, in many scientific papers, it is noted that porous rocks have a permeability hysteresis with a cyclic change in effective pressure. The researchers argue that the main cause of permeability hysteresis is the irreversible deformation that occurs due to compaction of the rock matrix. However, when studying the permeability hysteresis, due attention is not paid to related factors, such as the presence of colloidal particles inside the pore medium. Colloidal particles less than 1 μm in size can be natural, which got inside during the samples manufacturing, and also formed inside the pore space during destruction at grain contacts. All methods for determining permeability consist in establishing the flow rate of fluids through a rock sample under a pressure drop. When a gas or liquid moves, the colloids inside the porous medium also move and block the pore throats, while the permeability of the medium decreases. During filtration, the blockage of the pore throats occurs gradually, and therefore a slow decrease in permeability is observed, which is interpreted by many authors as creep.
In this project, we have developed a methodology to evaluate the contribution of colloid migration to the overall reduction in the permeability of core samples from effective pressure. The technique includes changings in the flow rate and direction. The research results showed that during filtration, colloids migration can lead to a decrease in core permeability by up to 50%, while an increase in effective pressure leads to a slight change in permeability. It was also found that with a cyclic change in the effective pressure, the permeability does not always show hysteresis, in contrast to classical laboratory studies. A comparative assessment of the effect of effective pressure on the porosity and permeability of core samples, as well as computed tomography data confirm the non-deformative nature of the decrease in permeability under cyclic loading. After a cyclic change in the effective pressure, the permeability was restored to its original values, while no visible violations of the matrix were found in the samples.

This work was supported by the RUSSIAN SCIENCE FOUNDATION, project no. 19-79-10034, https://rscf.ru/project/19-79-10034/.

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Energy Transition Focused Abstracts:

MS15 / **974**

Physics informed neural networks based on sequential training for CO_2 utilization and storage in subsurface reservoir

Authors: Kiarash Mansourpour[1]; Denis Voskov[1]

[1] *TU Delft*

Corresponding Authors: d.v.voskov@tudelft.nl, k.mansourpour@tudelft.nl

Simulation of CO_2 utilization and storage (CCUS) in subsurface reservoirs with complex heterogeneous structures requires a model that captures multiphase compositional flow and transport. Accurate simulation of these processes necessitates the use of stable numerical methods that are based on an implicit treatment of the flux term in the conservation equation. Due to the complicated thermodynamic phase behavior, including the appearance and disappearance of multiple phases, the discrete approximation of the governing equations is highly nonlinear. Consequently, robust and efficient techniques are needed to solve the resulting nonlinear system of algebraic equations. Machine learning (ML) techniques have recently been applied to a wide range of nonlinear computational problems. Recently, Physics informed neural network (PINNs) has been proposed for solving partial differential equations. Unlike typical ML algorithms that require a large dataset for training, PINNs can train the network with unlabelled data. The applicability of this method has been explored for the flow and transport of multiphase in porous media. However, for strongly nonlinear hyperbolic transport equations, the solution degrades significantly. In this work, we propose a sequential training PINNs to simulate two-phase transport in porous media. The main concept is to retrain neural network to solve the PDE over successive time segments rather than train for the entire time domain at once. We observe that sequential training can capture the solution more accurately concerning the standard training method. Furthermore, we extend the sequential training approach for compositional problems in which nonlinearity is more significant due to the complex phase transition.

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MS22 / **977**

Advancing modeling and simulation of batteries at different scales

Authors: Oleg Iliev[None]; Konrad Steiner[1]; Jochen Zausch[1]

[1] *Fraunhofer ITWM*

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The goal of this presentation is to highlight some of the recent developments of the Dept. Of Flows and Material Simulation from the Fraunhofer Institute for Industrial Mathematics in the area of modeling and simulation of batteries. The Department has a long history of academic research and

industrial projects on modeling, simulation and development of customized soft-ware of processes in batteries at different scales and complexity. Modern energy storage plays a key role in the course of rapid developement in renewable energy. Especially in the field of electromobility high demands like capacity, efficiency, endurance and security are made on the storage device, which are currently mostly Lithium-Ion-Batteries. The development of new materials for such improved energy storages is time- and money-consuming though. Hereby computer simulations can not only help to judge the performance of potential new battery cells, but to better understand the microscopical reasons. The latter leads to a more purposive and thus more efficient approach in the development of batteries. In this way, in particular, the for-mation of solid electrolyte interphase layer can be better understand, as well as the coupled electro-chemo-mechanical simulation processes.

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In-Person

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Poster / 978

Multiscale Direct Numerical Simulation of Pore Scale Fluid Flow Through Porous Media

Author: Gospel Ezekiel Stewart[None]

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Multiphase fluid flow through porous media has many beneficial applications for various industries such as oil and gas, hydrology, geothermal, medical, and manufacturing. A substantial amount of research has been carried out at various scales (e.g., reservoir, Darcy, microscale) to further understand the fluid behavior, with many recent studies directed towards the pore scale. This work has revolutionized our understanding of the fundamental principles governing fluid flow in porous media and their impact on larger scale applications. However, pore-scale investigation tools are not directly applicable to multiscale porous media (e.g., fractured, and microporous rocks or multi-layered membranes) because it is impossible to run simulations on an image of the domain that resolves all scales. The multiscale Darcy-Brinkman-Stokes (DBS) approach is a novel technique that has been gaining popularity in recent years that enables the inclusion of unresolved porosity in micro-CT images through Darcy parameters (e.g., porosity, permeability). The DBS approach has been successfully employed to investigate single-phase flow and reactive transport in multiscale porous media. DBS models for multiphase flow exist, but their capability to represent accurately capillary effects at the interface between scales is unclear. The main objective of this study is to evaluate the applicability of a multiphase DBS approach to simulate multiphase fluid flow through a multiscale porous medium. Simplified 2D models containing solid free regions and porous matrices are considered

and the results of DBS simulations are compared with the results of fully resolved simulations. The flow simulations are carried out using GeoChemFoam, our open-source pore-scale modelling solver package, in which the DBS method has been implemented. A wide range of regimes is considered and the domain of application of the DBS method is identified.

Participation:

In-Person

References:

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Vascular Design: Freedom, Evolution, Hierarchy

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Porous materials are usually thought of as amorphous mixtures of two or more things, solids, fluids, and voids. The research field started that way, and so did my own activity in it. Along the way, I was drawn to the part of nature (the physics) that was missing from the amorphous view: the structure, flow, configuration, drawing (design), purpose, and evolution.

The lecture is pictorial. It begins with defining the terms, because words have meaning: vascular, design, evolution, and prediction (theory). Next, vascular (tree shaped) architectures flow more easily than parallel channels with only one length scale (the wall to wall spacing). Transport across channels is facilitated when the spacing is such that the channel flow length matches the entrance (developing) length of the flow.

The tendency to evolve with freedom toward flow configurations that provide greater access is universal in nature, bio, and non-bio. This tendency is the Constructal Law, which empowers us to predict the evolution toward flow access, miniaturization, high density of heat transfer, and the scaling up (or down) of an existing design.

Vascular designs are icons of the design feature called hierarchy. Vasculatures occur naturally because they flow more easily than one-size designs. The movements in society are hierarchical, from city traffic to global air traffic, fuel consumption, and wealth. The future of evolutionary design everywhere points toward vascular, hierarchical flow architectures that will continue to morph with freedom and directionality.

To read more:

HEAT TRANSFER: Evolution, Design, and Performance, Wiley 2022.

FREEDOM AND EVOLUTION: Hierarchy in Nature, Society and Science, Springer 2020.

CONVECTION HEAT TRANSFER, 4th ed, Wiley, 2013.

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Porous Graphene Oxide Macrostructures for Water Treatment Applications

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Providing clean, safe water reliably in an affordable manner is a major global challenge. A wide variety of water pollutants, including heavy metals, dyes, pesticides, and pharmaceutical compounds pose a threat to public and environmental health. Existing water treatment technologies do not adequately meet water quality standards for removal of the diverse range of contaminants; thus, technological innovation is needed to enhance water security and accessibility. Engineered nanomaterials, such as graphene oxide (GO), offer tunable multifunctionality for effective removal of a diverse range of contaminants from water. However, the practical implementation of nanomaterials such as GO in water treatment requires their immobilization into three-dimensional macrostructures which may impair their performance. Unlike colloidal nanomaterials, solid macrostructures of GO can be easily stored, transported and manipulated. Despite the progress on forming high surface area and multifunctional GO macrostructures, synthesizing mechanically robust porous macrostructures, especially for wet applications, is a challenge. This talk will describe approaches for the preparation of GO-based macrostructures that can be used in water treatment. The functionalization of macrostructures of engineered nanomaterials with antimicrobials for prevention of biofouling or removal of pathogens from contaminated waters will also be discussed.

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Electroporation of cellular membranes for the enhancement of mass transfer in biological media: mechanism and technological applications

Author: Eugene Vorobiev[1]

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Cellular membranes serve as selective barriers for regulation of molecular transport between interior and exterior of cells. Under the effect of electric field pulses of very short duration (from several hundred of nanoseconds to several milliseconds) with pulse amplitude from 100-300 V/cm to 100-300 kV/cm, the biological membrane is electrically pierced and loses its semi-permeability temporarily or permanently. The electrical permeabilization of biological membranes (called electroporation) may be reversible or irreversible. It was shown that electroporation can serve to introduce into cells or extract from cells small and/or large molecules. This phenomenon has been applied to amplify the insertion of nucleic acid molecules in genetic modifications, to enhance drug transport in cancer treatment or for the killing of microorganisms. Electroporation can also be used to enhance extraction of valuable cell compounds (polyphenols, carbohydrates, proteins,..) from biological media (plant tissue and biomass materials). Biological tissue with electroporated cell membranes, but with a preserved cell wall network, is selectively permeable. For the purpose of mass transport, electroporated cell tissue presents a porous network with improved permeability and diffusivity characteristics.

This lecture presents the mechanisms of cell electroporation, its impact on the physical properties of biological media, and gives examples of mass transfer enhancement in electroporated cell network. Different methods to detect and quantify electroporation phenomena in porous network of biological tissue are presented. Impacts of electroporation on the mechanical, diffusional and electrophysical properties of biological media are illustrated by numerous examples. Physical models of liquid expression and compounds diffusion in compressible electroporated biological tissue are presented. Several innovative green technologies based on the pulsed electric energy induced electroporation are presented, including selective extraction, filtration, pressing, and drying of plant materials and biomass.

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Multi-Physics Repetitive Loads

Author: J. Carlos Santamarina[1]

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Most natural and engineered systems experience repetitive loading cycles of all kinds, including: stress (our bones and foundations), fluid pressure (the beating of our hearts, tidal action, and pumped hydro storage), suction (our lungs and natural dry-wet cycles), pore fluid chemistry (salt-water intrusion), and thermal cycles (such as silos, freeze-thaw, and geothermal systems). Repetitive loads can cause significant accumulations of volumetric strain (towards the terminal void ratio) and plastic shear strains (shakedown or ratcheting), lead to accelerated transport (of heat, chemical species and particles), and alter material properties and system performance. Complementary multi-scale experiments and simulations provide unique insights into the underlying mechanisms that explain the observed responses. Analysis and design must consider the influence of multi-physics repetitive loads on the long-term performance, serviceability and safety of engineered systems. Asymptotic trends can be used to obtain first-order estimates for simple boundary conditions; however, complex boundary conditions require numerical simulations, the development of new constitutive models and the implementation of hybrid algorithms that avoid standard time-stepping numerical protocols.

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Stability and functionality of immobilised liquid-liquid interfaces in periodic structured media

Author: Shervin Bagheri[1]

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In this talk, I will discuss how liquid-liquid interfaces can be stably locked into periodic structured porous substrates and used for controlling the transfer of momentum, heat and mass with an external flow. First, we address the behavior of liquid-liquid interfaces locked in textured surfaces and exposed to an external shear flow. When the liquid-liquid interface remains stable, these surfaces can enhance heat and mass exchange with a bulk flow and reduce flow drag and biofouling. We demonstrate how shear stresses and soluble surfactants modify the dynamics of the liquid-liquid interface, resulting in waves, drainage and Marangoni stresses, all of which significantly affect transport processes with the external flow. Second, we introduce systems with liquid-liquid interfaces locked in three-dimensional periodic porous scaffolds. By tuning the wettablity and introducing appropriate "fluid traps", we can immobilize interfaces of different morphologies, including spherical droplets or

diamond-shaped structures. These multi-phase materials are remarkably stable and provide a very high area-to-volume ratio. We will discuss their potential as flow-continuous heterogeneous catalysis and for other applications that require optimizing mass transfer across interfaces, such as CO2 capture.

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Magnetic Resonance Measurements of Fluids in Shale

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Shale formations are of increasing importance world-wide as petroleum reservoirs. Conventional core analysis measurements are ill suited to the analysis of shale samples since the pore fluids present are very difficult to extract due to the very small pore sizes. Magnetic Resonance (MR) permits non-invasive analysis of intact samples and is therefore an intuitively appealing method for shale analysis. The MR relaxation correlation measurement T1-T2 is now commonly employed for analysis of shale fluids. The T1-T2 measurement struggles to observe and quantify the fast decaying signal from pore fluids in shales. A new method, which we term T1-T2*captures the very short-lived fluid shale MR signal exceptionally well and provides well resolved discrimination and quantification of pore fluids, as well as the solid-like kerogen. In this lecture we will review MR relaxation time measurements of fluids in porous media, consider the broad category of MR relaxation correlation measurements ultimately leading to T1-T2* analysis of shales.

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987

Thermodynamic efficiency/limit of subsurface energy production/storage systems

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To mitigate the negative impacts of increasing CO2 concentrations in the atmosphere on climate change complementary decision tools should be considered when selecting or evaluating the performance of certain (sub-surface) energy production and/or storage systems. Here we explain the framework in which the subsurface energy system could be analyzed using the exergy concept based on the Second Law of Thermodynamics. The analysis considers the energy requirement of different stages in the life cycle of the considered system, which can later be used to quantify its CO2 emission. The exergy analysis provides valuable information on comparing different energy routes in terms of their end-to-end efficiency and/or their CO2 intensity (gr-CO2/MJ). We show application of the methodology for different hydrocarbon production systems, underground hydrogen storage, and CO2 capture and storage. We assert that during energy transition time the focus should be on minimizing CO2 intensity of the selected systems, regardless of its origin.

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Deep Learning for Parameterization and Calibration of Subsurface Flow Models

Author: Behnam Jafarpour[1]

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Calibration of subsurface flow models often leads to underdetermined inverse problems, where limited data is used to estimate spatially distributed hydraulic properties of geologic formations at high resolution. The problem is usually solved by using a given model of geologic continuity to

constrain the expected distribution and connectivity patterns of the solution. For non-Gaussian problems, imposing the specified model of continuity is not trivial. Low-dimensional parameterization methods are commonly adopted to improve problem ill-posedness and to capture and preserve the expected spatial connectivity patterns in the solution. Deep learning offers a new perspective for low-dimensional parameterization and calibration of complex high-dimensional flow models. Using training data with diverse and complex spatial connectivity patterns, deep learning models can learn a nonlinear mapping from high-dimensional spatial distribution of properties onto a low-dimensional latent space that provides a compact description of model calibration parameters. The resulting latent space can be used to parameterize the inverse problem and to facilitate the search for solutions that are geologically plausible and that reproduce the observed flow response data. More complex architectures can be developed by jointly constructing low-dimensional parameter and data latent spaces, and a direct inverse mapping from the data latent space to the parameter latent space, to perform regression. Alternative parameterization, inversion and data assimilation formulations that exploit latent space representations of model parameters and data are presented and discussed with examples to illustrate the performance of these methods.

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The Rheology of Granular Media: from Engineering to Geological Applications

Author: Raffaella Ocone[1]

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Granular materials exhibit a broad range of intricate dynamic behaviours. The study of their hydrodynamics is extremely relevant in the chemical and process industries, where those materials are widely handled and produced. Understanding how internal (e.g., particles size and shape) and external (e.g., applied stresses, moisture content) physical properties impact on the flow behaviour of solid particles helps industrial practitioners handle and produce particulates in an efficient and less costly way. Building upon previous findings applied to the process industry, the talk explores the challenges associated with the dynamic behaviour of dry and wet granular material and discusses recent experimental and modelling efforts on the flowability of pyroclastic powders. Pyroclastic powders are investigated with the aim of predicting and managing the hazard resulting from volcaniclastic debris flows, natural phenomena which occur when a mixture of pyroclastic fallout/current deposits and water move down slopes under the action of gravity.

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Finite element modelling of the growth and flow properties of multiple-scale three-dimensional fracture networks

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The generation and growth of multiple three-dimensional fractures, and fluid flow through the resultant fractured rock mass, is modelled by solving the displacement and flow equations numerically, using the finite element method. The approach uses the Imperial College Geomechanics Toolkit, an in-house C++ 3D simulator that captures coupled thermo-poro-elastic deformation and damage accumulation, while accounting for variable fracture apertures and local transmissivities on the fracture surface, which evolve as a function of deformation. Simulations are able to capture fracture growth at different scales, and model fracture nucleation based on the evaluation of a local damage model. Quasi-static fracture growth is simulated for a number of different stress regimes, making use of a new geometric representation of fractures, based on a novel periodic quadratic polynomial spatial B-spline approach. Surfaces are formed by lofting tip curves during fracture growth, resulting in a low-cost, high-resolution approach. Meshing of the domain uses quadratic quadrilaterals and hexahedra, as opposed to triangles and tetrahedra. The generated fractures are generally non-planar, due to the varying crack-tip stress intensity factors created by stress field interactions between neighboring fractures. Realistic three-dimensional fracture patterns emerge from the simulations, due to nucleation, growth, interaction and intersection of fractures at several scales. Datasets with thousands of geomechanically interacting discrete fractures at different scales will be presented. Fluid flow through the generated fractured rock mass exhibits interesting channeling effects, which are strongly influenced by the stress regime.

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How the Chemical Vapor Infiltration process can be optimized for the production of advanced composite and porous ceramics

Author: Gerard Vignoles[1]

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Chemical Vapor Infiltration (CVI) is a high-quality and versatile process enabling the preparation of reinforced porous and architecture ceramics as well as Ceramic Matrix Composites (CMC), which are high-temperature materials for aerospace, energy management and industrial systems. Very strong market growth perspectives trigger renewed interest in this process. However, being expensive and/or somewhat difficult to control and optimize, it needs modelling actions at least to provide guidelines for industrial usage.

This presentation will describe the process physico-chemistry and its modelling, which has to be multi-physics and multi-scale. The numerical tools range from simple analytical approximate formulae to detailed, image-based modelling of heat & mass transfer coupled to chemical reactions and featuring porous media with morphological evolution. Special attention is paid to (i) the relationship between fibrous media structure and transport properties, including rarefied gas transfer mode, (ii) the potential of using thermal gradients in order to optimise CVI and obtain a fast and efficient infiltration.

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Poster / 992

Investigation on the heat change during the disintegration process of pharmaceutical tablets

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Co-authors: Daniel J. Goodwin [2]; Ranjit M. Dhenge [2]; Joelle Nassar [2]; J. Axel Zeitler [1]

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[2] *GlaxoSmithKline*

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The disintegration process of pharmaceutical solid dosage forms refers to a mechanical break-up of an intact tablet into smaller fragments to enhance the drug substance's contact with the dissolution medium. This process is particularly critical for immediate-release dosage forms to ensure the end product's bioavailability and efficacy. Despite the significance of disintegration, the assessment methods specified by the regulators provide little scientific insight into the mechanisms of the process. This lack of insight is not surprising as the methods are very simple. However, tablet disintegration is a highly complex process due to the wide range of particle types being used, each exhibiting their own time dependence in swelling and dissolution behaviour and the impact of processes such as granulation or direct compaction. Previous studies have therefore focused on the micro-structure of the tablets by considering factors such as porosity, pore size distribution, pore connectivity, tortuosity, permeability, hydrophilicity, and so on for different pharmaceutical excipients and manufacturing conditions, but the mechanistic link to disintegration is not fully established yet 1.

In this study, we investigated the tablet's wetting process from a thermodynamic point of view by monitoring the temperature change of 1 ml of distilled water in which a sample tablet was immersed. In 1959 Claxton reported the observation of a temperature rise during spontaneous imbibition of a porous medium, which was explained by a decrease of free energy in the system [2]. Claxton's experiment, and subsequent studies, focused on the temporal and spatial evolution of released heat at the liquid front. Instead, we measured the total heat released during the wetting process as a function of time using an adiabatic chamber. As a result, we obtained different profiles of how temperature changes as a function of porosity in tablets of the same formulation. Measuring the temperature change of the dissolution medium showed potential as a novel approach to quantifying the hydrophilicity of complex compounds and estimating the liquid penetration into the porous media by analysing the correlation between the amount of heat released and the properties of the media.

Participation:

In-Person

References:

1 Alder, G., Frenning, G., 2022. Tablets and compaction, in: Aulton's pharmaceutics: the design and manufacture of medicines. Elsevier. chapter 31, pp. 406 501–541.
[2] Claxton, G., 1959. Detector for liquid-solid chromatography. Journal of Chromatography A, 2, pp.136-139.

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MS03 / 993

Particle-laden fluid flow in fractures: particle transport, deposition and clogging

Authors: Ahmed Hafez[1]; Qi Liu[1]; Thomas Finkbeiner[2]; J. Carlos Santamarina[3]

[1] *KAUST*

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Fluid flow through fractured rock masses determines groundwater resource utilization, contaminant transport and remediation, resource recovery (oil and gas, geothermal), and energy waste storage (CO2 geological storage). While the matrix determines storativity in most cases, fractures with high transmissivity control fluid flow. Fluid flow through fractures may be accompanied by particle transport, including detached native fines or injected proppants and lost circulation materials. Small-scale experiments fail to capture the radial-dependent inertial effects and particle clogging patterns that can emerge away from injection or extraction wellbores.

This research explores divergent particle-laden fluid flow through large-scale fractures. We designed and built a large-scale parallel-plate setup (diameter=900 mm) to mimic fractures with different surface topographies and apertures. The device is instrumented with multi-physics sensors, while the transparent plates facilitate real-time visualization and particle-tracking. We explore particles with different sizes, shapes and specific gravities (including quasi-buoyant and dense particles).

Experimental results, numerical simulations and energy-based analytical solutions highlight the development of an annular zone with negative pressure away from the central injection point (previously reported in very few publications in other fields). Annular depressurization is more apparent as the fluid flow rate increases, i.e., at high Reynolds numbers, and it is anticipated under field conditions during drilling (particularly while traversing high aperture fractures) or when imposing high fluid injection rates.

Quasi-buoyant particles follow the fluid streamlines. However, local changes in the fluid velocity field during radial flow can enhance particle retardation, which changes the local particle concentration and enhances the probability of clogging. Dense particles transported along horizontal fractures settle to form an annular "dune"during divergent radial flow. Experimental and numerical results show the interplay between particle concentration, fracture aperture and injection flow rate on the dune topology and its radial distance to the injection port. Particle deposition patterns and the resulting dune topology become more complex in fractures with rough surfaces or shear-induced anisotropic transmissivity. Analytical and numerical studies investigate the relative role of the various parameters involved.

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MS06-A / 994

Droplets at Liquid-Fluid Interfaces: Pressure Field and Coalescence

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When a water droplet falls through oil to reach the interface above a water layer, it can remain at the interface for a prolonged time until coalescence takes place. A similar situation takes place when an oil droplet ascends through a water column and reaches the interface beneath an overlying oil layer. Several parameters affect the characteristic time to coalescence, including temperature, viscosity, relative densities and solubility. The purpose of this study is to gain further insight into the underlying mechanisms leading to coalescence.
We photograph droplets as they approach the liquid-liquid interface to assess the droplet and interface deformations; in particular, we obtain undistorted images of the droplet at the interface by matching the refractive index of silicone oil and a water-glycerol mixture, and determine the differential fluid pressure from continuous curvature measurements around the droplet (Young-Laplace). Results show that the droplet and the interface interact through the fluid pressure within the thin film that separates them; consequently, the droplet and the interface deform each other. Away from the interface, the droplet curvature responds to the interfacial tension between the two fluids; at the interface, the droplet curvature is proportional to ~2 because of the double-surface structure of the thin film. More precisely, curvature measurements reflect the pressure gradient that drives fluid drainage within the liquid film and eventually leads to coalescence. Complementary observations show that an initially curved oil-water interface extends the time to coalescence (longer drainage path), confirm "dimple"formation at the interface (depends on viscosity), show droplets bouncing at interfaces (when they approach it with high terminal velocity), and indicate complex mutual interactions when multiple droplets reach the interface quasi-concurrently.
These results are relevant to a wide range of liquid-liquid and liquid-gas systems, such as emulsions, drug delivery, food preparation, cosmetics, painting, oil recovery, oil-water separation, offshore contamination, LNPL and DNPL migration, and augmented sealing capacity for geological CO2 storage.

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MS04 / 995

Poromechanics of a yeast aggregate placed under fluid constraints

Authors: Térence Desclaux[1]; Pierre Joseph[2]; Paul DURU[3]; Morgan Delarue[2]; Olivier Liot[3]

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The capture of solid particles in a porous medium is critical for many processes but has a major drawback: internal fouling due to pore clogging. Clogging at pore scale is now well understood for inert and rigid particles, but the study of bio-clogging - clogging by biological objects, e.g. living cells - opens many topical research questions as living cells have particular properties that may impact the clog properties: they are deformable, endowed with specific adhesion mechanisms, and are able to proliferate. As a result, these cells can both change their shape and volume, leading to local cellular rearrangements, thus modifying the microstructure of the clog, and consequently its hydrodynamic resistance. In the literature, this change of hydraulic resistance has been extensively studied at the macroscale (the scale of a membrane, the whole clog). In particular, it has been reported that the resistance of a clog depends on the hydrodynamic pressure imposed to the filtration system. But the precise interpretation of this phenomenon is still controversial and patchy: observations are missing at the microscale (the pore, the cell). In particular, a precise understanding of displacements and rearrangements inside a yeast clog, and a link with the local microstructure is still missing.

To address this specific issue, we have developed an experimental quasi-2D microfluidic device consisting in one single pore retaining cells whose properties are well known and easily controllable: the baker's yeast Saccharomyces cerevisiae. After an initial build-up phase, the pressure driving the flow through the pore is changed in order to compress/decompress the clog cyclically, while the flow rate is measured and the clog is imaged under an epifluorescence microscope. This allows to directly measure the microstructure from nucleus fluorescence (figure, center panel), and to quantify the movements within the clog (bright field microscopy, figure, left panel), using dedicated algorithms to distinguish collective movements and local rearrangements (figure, right panel).

These results provide the first observations of the compressibility of a yeast clog at the microscale, and reveal that, in the absence of proliferation, the clogs undergo a first compression with plastic-elastic deformations, characterized by both large collective displacements and local cell rearrangements, while the following compressions are characterized by smaller deformations that are mainly elastic. The plastic deformations modify the local microstructure, as the clogs are denser after compression/decompression cycles than before. Finally, the hydraulic resistance of the clog increases with the hydraulic pressure.

Together, these results show a poromechanical fluid-structure coupling: the fluid deforms the porous medium which in turn modify the fluid percolation. They also show several quantitative differences with the predictions of poroelasticity theory. A dedicated DEM model has thus been developed, to simulate the mechanical behaviour of individual yeast cells. Simulations reproduce quantitatively well the experimental results, which suggests the discrepancies with the poroelasticity theory come from the particle/particle and particle/wall friction.

Overall, this study presents the first measurements of the poromechanical behaviour of a yeast aggregate, and suggest that it is significantly altered by the specific adhesion mechanisms of individual cells.

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In-Person

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Energy Transition Focused Abstracts:

MS22 / **996**

Direct fabrication of porous 3D microstructures on silicon wafers for MEMS applications

Authors: Olaf Andersen[1]; Cris Kostmann[1]; Thomas Lisec[2]; Thomas Weißgärber[3]

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A new automated method for the fabrication of functional 3D porous structures directly on planar standard silicon wafers has been developed [1,2]. A typical approach comprises the filling of a mold pattern with micron sized particles of the desired material, and their fixation via atomic layer deposition (ALD). It has been demonstrated that it is possible to manufacture for example micromagnets from NdFeB powders that can be used for energy harvesting.
In order to achieve smallest dimensions and highest filling factors, the utilization of dry powder as the starting material is beneficial. The new approach utilizes the superimposition of high- and low frequency oscillations for particle mobilization in order to achieve optimum mold filling. Additionally, rubber balls are applied for densification of the powder packing.
For verification of the application properties, micromagnets were created from 5 µm NdFeB powder on 8”Si wafers, using the novel automated mold filling technique, as well as an existing manual one for benchmarking purposes. Subsequent atomic layer deposition were utilized to agglomerate the loose NdFeB particles into rigid microstructures. The magnetic properties and inner structure of the NdFeB micromagnets were investigated. It is shown that the novel automated technique outperforms the manual one in major terms. In addition, examples for further materials and applications will be briefly discussed.

Participation:

In-Person

References:

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MS01 / **1000**

Ostwald Ripening Investigation using 3D Micro-CT Imaging

Authors: Waleed Dokhon[1]; Yihuai Zhang[2]; Martin Blunt[3]; Branko Bijeljic[4]

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The goal of reducing carbon emissions relies heavily on the world's energy sectors to undergo significant energy transformations. The hydrogen economy plays a critical role in achieving that goal by harvesting hydrogen and using it as an energy carrier. The current storage options limit hydrogen's large-scale adaptation to a major energy form. For that reason, underground hydrogen storage has been an alternative that appealed to the scientific community and prompted multiple studies to explore its feasibility in several aspects. One of those aspects is evaluating the potential of remobilising trapped gases in a porous medium through the Ostwald ripening phenomenon. As such, we examined the phenomenon of Ostwald ripening by leaving the H2-brine system in a sandstone sample uninterrupted for 12 hours to observe any hydrogen re-distribution. The sample was scanned with a micro-CT twice: before and after. Additionally, we demonstrated the derivation of a simple equation that estimates the timescale for disconnected gas ganglia to reach partial equilibrium over a given length scale. Finally, we explored whether changes in the interfacial curvature, in-situ contact angles, saturation distribution, and gas ganglia size distribution occurred during the 12 hours.

We observed the re-distribution of gas ganglia and the emergence of multiple larger new gas ganglia with a maximum extent of about 2 mm. This confirmed the length scale estimation made by the derived equilibrium timescale equation. Additionally, a slight increase in curvature was observed after 12 hours, and the mean contact angle slightly increased at the bottom part of the sample. Overall, our experimental study of the Ostwald ripening phenomenon presented significant remobilisation of trapped gas ganglia and gas re-distribution at the pore scale, which could mean that residually trapped hydrogen can be less than what is thought.

Participation:

In-Person

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1001

Permeability damage and restoration in porous media due to clay migration during fresh water injection

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The permeability decline in natural porous media due to clay mobilization is a problem of interest in several subsurface engineering applications such as oil recovery, water disposal, and carbon storage. When fresh water is injected into porous media containing resident brine, the sudden change in salinity causes the native clay fines to mobilize and clog pore spaces, resulting in a sharp decline in permeability. The mobilization of the clay fines is attributed to the weakening of the Derjaguin-Landau-Verwey-Overbeek (DLVO) forces that bind them to the grain. Khilar and Fogler (1983) studied the cyclic injection of fresh water and brine into a Berea sandstone core, and found that the permeability damage after fresh water injection in a given direction is not restored when followed by brine injection in the same direction. However, injecting brine in the opposite direction restored the permeability damage. These findings indicate a dependency of the permeability damage on the immediate history of the flow, in addition to the salinity of the fluid.

Constitutive models of permeability in the presence of clay fines for field-scale simulations should reflect this phenomenon, and pore-scale analyses of clay mobilization are a powerful tool to build said models. In the current work we carry out 2D pore-scale simulations of cyclic fresh water and

brine injection into a porous medium containing non-swelling clay fines. We consider a sandstone-based porous medium of porosity 0.37, containing kaolinite with a clay mass fraction of 2%, and in each cycle, we sequentially inject: brine forward, fresh water forward, fresh water backward, brine backward, and brine forward. The brine salinity is 0.1M and the fresh water salinity is 0.001M. The pore-scale simulations are carried out using an in-house CFD code that employs the immersed boundary method to model clay-liquid and grain-liquid interactions. The code also accounts for the clay-clay and clay-grain DLVO interactions. We present the permeability damage during the cycle and the permeability restoration at the end of it.

Our ensemble averaged results from six randomized realizations of the porous medium with a uniform clay size of 3 micron, and a grain size of 20 micron, show that the permeability decreases by two orders of magnitude during forward fresh water injection compared to forward brine injection. When the fresh water flow is reversed, there is a momentary restoration in permeability followed by a sharp decline. The permeability damage is not restored when brine is injected in the backward direction, but is 99% restored when followed by brine injection in the forward direction. These trends are consistent with Khilar and Fogler (1983)'s observations, and confirm the mechanism by which clay fine mobilization affects permeability. Additionally, we present simulations of the cyclic fresh water and brine injection with a non-uniform clay size distribution. For a fixed mean clay size and clay density we observe that the non-uniform size distribution results in a lower permeability damage compared to the uniform size case.

Participation:

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References:

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1002

Method and Application for Judging Critical Temperature of Heavy Oil Rheology

Authors: Jinto Wu[None]; Guangming Pan[None]; Hao Li[None]; Jifeng Qu[None]; Yang Lijie[None]

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By laboratory experiments, the heavy oil rheology is confirmed to has a critical temperature. Above the critical temperature, the heavy oil exhibits Newtonian fluid properties; under the critical temperature, the heavy oil exhibits Bingham non-Newtonian fluid properties. According to the mechanism of viscous flow activation energy reflecting the rheological changes of heavy oil, a critical temperature discrimination method for heavy oil rheology was established. Based on the viscosity-temperature relation experiment data of crude oil, the relationship between lnμ and 1/T is plotted. The curve has obvious inflection point. At the inflection point, the viscous flow activation energy changes. The heavy oil is converted from Newtonian fluid to non-Newtonian fluid. The corresponding temperature of the inflection point is critical temperature. The practicability of the method was verified by the heavy oil data of Bohai L Oilfield and Liaohe Lengjia Oilfield. By using this method,

the critical temperature of heavy oil in well region 6 and well region 7 of Bohai N Oilfield is discriminated, which provides a basis for the formulation of thermal injection parameters in the preparation of thermal recovery development plan.

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Energy Transition Focused Abstracts:

1003

Research and Practice of Enhanced Production Control in Offshore Ultra-High Water Cut Oilfield

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After more than 20 years of water flooding development in Bohai K Oilfield, the remaining oil after entering the ultra-high water cut stage is highly dispersed, and it is increasingly difficult to stabilize production rate. In order to improve the development effect of the oilfield, the method of enhanced production control is proposed. For the parts with low permeability and poor water driven utilization in the formation, the inherent balance of oil and water migration can be broken and the degree of water driven utilization can be improved by increasing the production pressure difference, so as to alleviate the contradiction in the formation in the later stage of water flooding development. Based on the analysis of the relationship between the driving pressure gradient and the starting pressure gradient under different permeability, from the perspective of effective utilization of low permeability reservoirs, the relationship chart of reasonable production pressure difference and mobility under different well spacing is established. Using this chart, it is proposed that the production pressure difference of Bohai K Oilfield should be increased from 2.0MPa to 5.0MPa. This method has achieved good practical results in this oilfield. The water cut of a single well has decreased and the oil production has increased. The production of the oilfield has been stable for five consecutive years and the oil recovery has increased by 4%. This method can provide reference for the development of similar oilfields.

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Energy Transition Focused Abstracts:

1005

Pore-scale characterization and modeling of heterogeneous shale samples based on deep learning

Authors: Yuqi Wu[None]; Keyu Liu[1]; Chengyan Lin[1]; Chunmei Dong[1]

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Accurate prediction of the physical properties of heterogeneous porous media based on digital models requires 3D high-resolution (HR) and large-scale images. It is, however, extremely challenging to acquire such images since the current imaging technologies cannot resolve the dilemma between the high resolution and large field of view and we often end up with low-resolution images but with a large field of view or HR images with a small field of view. Moreover, available HR images are limited and always unpaired with accessible low-resolution images. Therefore, we proposed a hybrid unsupervised end-to-end deep learning method to fuse the fine-scale structures from 2D HR images into 3D low-resolution CT images for reconstructing 3D HR and large-scale digital rocks based on limited unpaired training images. The presented method is accurate since the porosity, pore size distribution, multiple-point correlation, and permeability of the reconstructed digital rocks are in good agreement with laboratory measurements.

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Energy Transition Focused Abstracts:

Poster / 1006

Remediation of multilayer soils contaminated by heavy chlorinated solvents using biopolymer-surfactant mixtures

Authors: Amir Alamooti[1]; Stéfan Colombano[2]; Azita Ahmadi[3]; Hossein Davarzani[4]

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The remediation of contaminated soils is an environmental critical issue. A common form of contamination is caused by heavy chlorinated solvents spills, commonly used in industrial processes 1. Also, remediation is particularly challenging when these pollutants are present in multi-layered soils [2]. A promising approach for the treatment of these soils is the use of polymer solutions [3]. Although polymer solutions can improve the remediation of these pollutants, the residual pollutant after the flushing can still be noticeable. Surfactant solutions can improve the recovery of pollutants by surface tension reduction; however, their efficiency in multilayer systems is limited [4]. Combining polymer and surfactant in a mixture can result in a remarkable improvement in the recovery of the pollutant [5].

In this work, experimental and numerical approaches are used. Xanthan as a biopolymer and sodium dodecylbenzene sulfonate (SDBS) as a biodegradable surfactant are used. To study the interactions between the polymer solution and surfactant, various tools such as rheometer, and scanning electron microscope (SEM) are employed. 1D-column experiments have been used for both single-phase and two-phase flow. To evaluate the performance of the polymer solutions in the remediation of chlorinated solvents in a multilayer system, a decimetric-scale 2D sandbox is used. Two-phase flow in multilayer porous media is simulated to understand the underlying physics behind the experimental results. The continuity equation is coupled with generalized Darcy's Law and the non-Newtonian behavior of the polymer solutions is incorporated into the model.

The xanthan solution exhibited shear-thinning behavior. However, when mixed with SDBS, the viscosity decreased with no correlation between the viscosity of the mixture and the concentration of the surfactant, given a constant concentration of xanthan. This is attributed to the mutual electrostatic repulsive forces and hydrophobic interactions confirmed by SEM images. The analysis of two-phase flow in a 1D-column indicates that incorporating a surfactant in the polymer solution leads to higher recovery efficiency for 15%. Furthermore, the flow of the polymer/surfactant mixture when using a mixture of polymer and surfactant, the flow of pollutants after breakthrough lasts longer and the pressure difference along the column is lower compared to using the polymer solution alone. The experiments in the 2D system illustrate similar results, the higher recovery and lower differential pressure for the mixture of polymer/surfacatant. Another important feature of the 2D experiments is the density-driven flow of the polymer/surfactant solution in the multilayer system. The multilayer experiments for the polymer and heavy pollutants flow visually demonstrate that the density, as well as permeability differences between the layers, have an impact on cross-flow. The simulation of multiphase flow in a multilayer system produced results that matched well with those from the experiments. The simulation results also reveal that if the upper layer in the 2D system is not confined, the polymer solution as the lighter fluid moves mainly vertically. To address this, a set of experiments were conducted in a larger 2D system with a horizontal well injecting a blocking agent, which successfully prevented the vertical movement of the polymer solution.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS13 / **1007**

Structure and adsorption mechanisms of hydrogen gas on water-saturated montmorillonite clay: A molecular dynamics study

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Radioactive waste arising from the production and use of radioactive materials calls for a sustainable waste management system which guarantees long-term safety to human and environment. To this end, a multi-barrier deep geological storage system consisting of both natural geological formations and engineered barriers has been proposed by several countries as a viable concept to store intermediate and high level wastes [1-3]. One of the central issues in the quantitative assessment of the integrity of a deep geological repository is gas generation and migration. Hydrogen (H_2) gas, resulting from the anaerobic metal corrosion and water radiolysis processes is the most significant gas expected after the closure of the facility. Clay minerals, which are abundant in these geological sites, exhibit an intricate atomic structure with different polar species able to interact with H_2 gas. In this study, we explore the structure and energetics of H_2 gas adsorption on the interlayer, basal and edge surfaces of a montmorillonite clay model using molecular dynamics simulations. A special focus is given on the effects of local compositional and structural heterogeneity of montmorillonite. The simulation results show that on the basal surfaces, H_2 occupies the siloxane cavities with the Al/Si isomorphic substitutions on the tetrahedral sheet limiting the occupation of those sites. A detailed analysis on the edge surfaces reveal that the local structure of water governs the adsorption energetics of H_2 on the edges and within the interlayer pores.

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Energy Transition Focused Abstracts:

MS23 / 1008

Colloidal particles adsorption fluctuations: experimental and kirkwood buff integrals approaches

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Colloidal particles (amidine latex, 1 µm in diameter) in aqueous solution are put in contact with a glass slide under ambient conditions where they adsorb. The particle concentration is fixed during the experiment by mean of an infinite reservoir. Using a simple optical microscope, 240 x 320 µm2 images of the population of the adsorbed particles are taken while the glass slide and the solution are at equilibrium. Analyzing the surface population we get the direct access to the isotherm, i.e. surface concentration as a function of solution concentration. The isotherm is alternatively obtained both from the density fluctuation and/or from the pair distribution function and the use of the Kirkwood Buff Integral. The results clearly show the equality of the chemical potential between the two phases.

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Energy Transition Focused Abstracts:

MS23 / 1009

A (dual) network model for heat transfer in coupled porous media free flow systems

Author: Rainer Helmig[1]

Co-authors: Timo Koch [2]; Martin Schneider [1]; Anna Mareike Kostelecky [3]; Helge Dahle [4]; Johannes Müller [1]; Bernhard Weigand [1]

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Heat transfer processes and non-isothermal effects are found in many technical and environmental coupled porous-media free flow systems.
Prominent examples including two-phase flow range from fuel-cell water management and food drying to soil evaporation and salinization. Modeling these types of systems is challenging due to the variety of length and time scales involved and the high physical complexity of the processes

In this work, we introduce a fully coupled, locally energy- and mass-conservative dual network model for the simulation of heat transfer in realistic natural porous media, allowing the consideration of pore-local thermal non-equilibrium and structural heterogeneity coupled with a free flow system . Energy transfer in the dual network is modeled as a fully coupled processes using pore and grain-local heat transfer rules derived from the analysis of local idealized but spatially resolved problems and geometrical considerations. he solid space. Both porous media subdomains are simplified using the same model reduction technique commonly applied exclusively to the void space, where it is known as pore-network modelling.

Using selected examples, we will show the conditions under which thermal non-equilibrium plays a role.

Participation:

In-Person

References:

Weishaupt, K., R Helmig (2021). A Dynamic and Fully Implicit Non-Isothermal, Two-Phase, Two-Component Pore-Network Model Coupled to Single-Phase Free Flow for the Pore-Scale Description of Evaporation Processes. Water Resources Research 57 (4),

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Koch, T.; Weishaupt, K.; Müller, J.; Weigand, B.; Helmig, R. (2021): A (Dual) Network Model for Heat Transfer in Porous Media. Transport in Porous Media, 1–35

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1010

Characterization method of wettability of tight sandstone of digital core based on CT scanning

Author: Jing Yu[None]

Co-authors: Zhongnan Wang [1]; Keyu Liu [2]

[1] *Research Institute of Petroleum Exploration and Development*

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The wettability of reservoir rocks is an intrinsic property that affects the behavior of fluid flow through porous media. The wettability of rocks in tight sandstone reservoirs affects the occurrence state and location of oil in pores. However, quantitative measurements of wettability are difficult to accurately characterize in tight sandstones. In this study, we measured the contact angle of dense sandstone using micro-CT image analysis and analyzed the distribution of oil and brine in the pores of the rock and the wettability of the rock.

The experimental steps are as follows:

1. Select rock samples with good physical properties and samples are cleaned to remove oil, and then the 3D CT data volume of the dry rock sample is obtained by micron CT scanning;
2. The sample is then saturated with brine doped with 10% NaI as a contrast agent, and crude oil is injected to displace the brine to the bound water state. The core is immersed in the crude oil to restore the wettability of the sample to the original reservoir state;
3. The brine with 10% NaI is used to displace fluids in the core plugs. The displacement of the brine would attain 30 PV (pore volume). And then micro-CT scanning would be conducted again to obtain the 3D X-ray CT data volume of the saturated mini-plug sample with oil and brine;
4. The CT data volume obtained is processed using the Avizo software. The CT data volume of dry rock samples can be processed to obtain the three-dimensional morphology of pores;
5. On this basis, according to the difference of CT values of different fluids in the pores, the oil is black, the brine with the contrast agent is dark gray, and the rock skeleton is light gray, the segmentation threshold was set according to the gray distribution. Brine, oil and rock skeleton were obtained after 3D CT images of rocks saturated with oil and water were segmented;
6. The methodology for measuring the contact angle is as follows. Select the image of oil and water coexistence in the pore, observe the distribution characteristics of oil and water, and measure the contact angle between oil and solid space in the pore.

Conclusions：

In this study, the contact Angle of oil in the pore of sample 1 is between 115.13° and 155.29°, with an average value of 135.81°, indicating that sample 1 is a hydrophilic rock. The contact Angle of oil in the pore of sample 2 is between 30.58° and 75.98°, with an average value of 54.54°, indicating that sample 2 is an oil-wet rock. In pores of oil-wet rocks, oil is attached to the surface of porous rocks in the form of film or dispersed liquid droplets occupying the edge of the pores, while brine occupies the centers of pores. In pores of water-wet rocks, brine mainly occupies the corners of pores, enclosing oil in the form of droplets or films.

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Energy Transition Focused Abstracts:

1011

A Comparison of the Flow of Foam, Gel and Foam-Gel in Carbonate Cores

Authors: Jinxun Wang[1]; Lyla Almaskeen[1]; Abdulkareem AlSofi[1]; Ming Han[1]

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In petroleum industry, formation heterogeneity is often observed in many oil reservoirs, which impairs the efficient sweep of oil by waterflooding. In such reservoirs, conformance control is essential to ensure the injected water or chemical solutions optimally contact the remaining oil with minimal throughput. Foams and gels have been applied as fluid diverting or blocking agent to improve oil displacement efficiency in many reservoirs. Combining foam and gel for conformance application also attracted attentions in recent years. With limited studies for high temperature and high salinity carbonates, the careful laboratory evaluation of the transport of these chemicals in carbonates is essential for screening reliable agents to achieve successful field applications.

In this study, we performed a comparative evaluation on the potentials of foam, gel and foam-gel for high temperature carbonates. Bulk tests were used for initial screening. Foam heights were used to screen foaming agents. A wide range of foam-gel solutions were prepared with different polymer types and polymer concentrations to study gelant effect on foam stability. The effect of foamer on gelation was evaluated through bottle tests. Based on the results, an optimal concentration ratio of gelant to foamer was determined and used in core-scale displacements to further study the potential of this hybrid foam-gel process.

Coreflooding experiments were performed at high temperature and high pressure conditions to evaluate the achieved and sustained mobility reduction (resistance and residual resistance) for different conformance control processes, including foam, foam-gel and gel. Results showed that compared to the water/gas co-injection, foam provided no additional resistance factor (RF). However, injecting foam resulted in higher and more sustainable residual resistance factor (RRF). Foam-gel injection exhibited higher RF and RRF values than the foam process, while the conventional gels showed even higher RF and RRF values than foam-gels. Relatively lower RRF was achieved by the foam-gel compared to the gel treatment, indicating that the foam-gel treatment might be less effective when strong blocking is required (for example, extremely high permeable regions). However, combining two of the most widely used conformance control methods (foam and gel) can strike a balance. The foam-gel tends to be more easily delivered than pure gelants, and the stability is significantly improved compared to the pure foam. Foam-gel may offer a treatment that is deeper and more sustainable than foams, while the treatment is more practical and cost effective than gels. Results of this study also demonstrate that such synergetic conformance control can be achieved in high salinity and high temperature carbonates with pronounced impact.

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Online

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Energy Transition Focused Abstracts:

Poster / 1012

Mono-energetic Micro-computed tomography(μCT) A reliable potential alternative to mineral Investigation of formation rock

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Traditional mineral investigation techniques are normally destructive and although they provide very useful information, they come with disadvantages and limitations some of which cannot be ignored. A case in point is the mechanical damage in the preparation process of SEM scanning during which artifacts will be introduced to the results. Micro-computed tomography (μCT) in combination with Finite Element Analysis (FEA) based simulation provides a unique opportunity to develop a non-destructive analysis tool. The workflow is as follows:
First, the μCT provides a voxel-based image. Using the already commercial software, this image can be translated into a 3D digital version, meaning that the pore-throat network and the grain structure are modeled and mapped digitally. At this point, porosity, permeability, pore size distribution, capillary pressure and etc are the deliverables. To Apply a structural analysis, a mesh can be created using the geometry of the sample. This mesh can then be used by a finite elements simulator to simulate mechanical properties like strength. The Application of Random field theory is necessary to count for the heterogeneity of the sample.
As for mineral detection,here we have used monoenergetic μCT. The novelty of the technique is to scan some reference materials alongside the sample. There are some subtle points to consider in the choice of the reference material, for example, the density of the reference materials should be distributed alongside the histogram.
Since the density(ρ) of the reference materials is known, the intensity(⊠) and the pertaining standard deviation can be easily calculated which will be used to correlate a particular density to intensity. Using the histogram, the count for the calculated intensity is the volume of the related density. This volume can again be converted to weight percentage using density.
Important to note is that before applying this technique a database must be created that includes the mineral phases/groups we are expecting. Here, this was done by scanning and analyzing three samples. The minerals in the fourth sample then was predicted using the μCT and was compared afterward with the XRD results. A good similarity is found.
The Differences could be owing to the presence of different mineral groups with similar densities. This problem can be addressed by considering more elements (for example topological factors) into consideration. Moreover, we can increase the accuracy of the (⊠, ⊠) function by using more reference materials.

Conclusion

As a proof of concept, a simple yet relatively accurate method is described here to confirm that minerals can be identified by mono-energetic μCT. To do so, an initial database was necessary. Using four reference materials with known densities, a regression model was used to correlate the pixel intensity with the density of the reference materials in the first step and with the density of minerals in the second step. Afterward, by using the frequency (counts in the histogram), the minerals abundance was quantitatively calculated for a new sample that was not used for the development of the model.

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1014

Partial Molar Properties from Single Molecular Dynamics Simulations

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It is shown how to compute partial molar properties (e.g. partial molar volumes, energies, and enthalpies) of fluid mixtures from single Molecular Dynamics simulations in the microcanonical or canonical ensemble, using only relatively simple post-processing of trajectories. The method uses least squares linear regression of local fluctuations of particle numbers and energies in combination with the Small System Method, and is in principle valid for any number of components and for any type of intermolecular interactions. For multicomponent systems, only a single simulation is needed for a given composition of the mixture. Simulations of a binary WCA mixture are used to illustrate the method, and to investigate the effect of system size. This approach has some practical advantages over the Kirkwood-Buff approach.

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Nanoscale interface dynamics: Self-assembly and stability of interface film of multi-phase flow in porous media

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[1] *University of Oslo*

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Self-assembly phenomena have been observed widely in the interface of multi-phase flow in porous media. Surfactant or surfactant-like particles play an important role during the self-assembly process. In this work, we employed a series of molecular dynamics simulations to investigate the self-micro emulsification and formation of self-assembly nanoparticle film. Atomistic insights into the self-micro emulsifying process and the underlying mechanisms are crucial for the design and tuning of the size of microemulsion droplets toward applications. Coarse-grained models were used to explore the role that droplet sizes played in the preliminary self-micro emulsifying process. The time evolution of liquid mixtures consisting of several hundreds of water/surfactant/oil droplets was resolved in large-scale simulations. By monitoring the size variation of the microemulsion droplets in the self-micro emulsifying process, the dynamics of diameter distribution of water/surfactant/oil droplets were studied. The underlying mass transport mechanisms responsible for droplet size evolution and stability were elucidated. Specifically, temperature effects on the droplet size were clarified. As a continuous task, the self-assembly behavior of amphiphilic nanoparticles was studied, and the mechanical properties of the interface film has been measured. This work provides knowledge of the self-micro emulsification of water-in-oil microemulsions at the nanoscale and the formation of nanoparticles film. The results are expected to serve as guidelines for practical strategies for preparing a microemulsion system with desirable droplet sizes and an expected interface film consisting of nanoparticles.

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In-Person

References:

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Energy Transition Focused Abstracts:

1018

Modeling non-equilibrium thermodynamics of cell membranes with lattice Boltzmann methods

Author: James McClure[1]

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Corresponding Author: mcclurej@vt.edu

The cell membrane plays a crucial role in supporting the energetic operations of biological systems. Cells are amazingly energy efficient, relying on mechanisms to process and store energy that evolved over hundreds of millions of years. Understanding and harnessing these mechanisms will be a key to developing the next generation of biotechnologies. Within this context, the movement of ions determines the electronic structure of the cell membrane and controls many aspects of the non-equilibrium response. Depending on the particular process, hundreds to thousands of membrane proteins may be involved in controlling these effects. Whole cell models provide a way to directly resolve these physics as a way to predict membrane responses and inform engineering approaches that target membrane transport. In this talk I will describe a new approach to model cell membrane transport problems using lattice Boltzmann models. I will highlight examples where whole-cell computational models can provide a way to understand how cell structure influences thermodynamic efficiency in biological systems.

Participation:

Online

References:

JE McClure, Z. Li "Capturing membrane structure and function with lattice Boltzmann models" arXiv:2208.14122

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1019

Key points to be paid attention to in unconventional oil and gas porous flow experiment

Authors: zhengming yang[1]; Xinli Zhao[2]; Yutian Luo[None]; Haibo Li[None]; yapu zhang[None]

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The unconventional oil and gas (shale gas, shale oil and tight oil, et al.) revolution has supported the rapid rise in oil and gas production in the United States. China is rich in unconventional oil and gas resources, which will be the main body of the company's current and future production. However, the unconventional oil and gas development is not effective, so it is urgent to explore new development methods. These new development methods depend on the research of physical simulation experiment technology. Therefore, this paper discusses problems that need to be paid attention to in the physical simulation experimental of unconventional oil and gas porous flow mechanism. Firstly, the unconventional oil and gas reservoirs are distributed continuously in a large area, but their heterogeneity is strong. Are the cores obtained in experiments representative? For example, On the one hand, shale oil can be divided into three types: interbedded type, lamellar type and pure shale type. The representativeness of the cores obtained from each type of shale oil has an important influence on the results. On the other hand, shale gas reservoir has strong vertical heterogeneity,

which requires high target location, and plane heterogeneity leads to large productivity difference of single well. Hence, obtaining representative shale core samples is of great significance for planning and improving production. Secondly, the unconventional oil and gas reservoirs require volumetric fracturing. What is the fluid flow mechanism under such conditions? Taking shale oil as an example, it is necessary to explore how to exert pressure imbibition and spontaneous imbibition to improve the development and production effect of shale oil. Finally, the large-scale development of unconventional oil and gas was achieved through "horizontal well + volumetric fracturing" in the early stage, but the investment was large and there was little room for adjustment of well pattern in the later stage. How to improve the development effect? Similarly, the primary recovery time of shale oil development is short and the secondary recovery effect is poor. The concept of enhanced oil recovery (EOR) needs to be integrated into the experimental design of unconventional oil and gas development to improve the performance of shale oil.

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Energy Transition Focused Abstracts:

MS23 / 1020

Dynamic contact angles and dynamic regimes for advancing liquid fronts

Author: Ignacio Pagonabarraga[1]

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Flocks of birds, schools of fishes, or bacterial colonies constitute examples of living systems that coordinate their motion. In all these systems their constituent elements generate motion due to energy consumption and can exchange information or react sensitively to chemical cues in order to move together or to react collectively to external signals. Artificial systems, such as Janus colloids, exploit the heterogeneous compositions of their surface to displace as a result of the heterogeneous chemical processes that take place in the presence of appropriate chemical substances.
All these systems are intrinsically out of equilibrium in the absence of any external driving. Therefore, their collective behavior emerges from a balance between their direct interactions and the indirect coupling to the medium in which they move, and a self-consistent dynamical approach is required to analyze their evolution. The mechanical balance that determines their collective behavior makes these systems very versatile.
Synthetic active particles constitute a class of model systems with huge technological potential.
I will analyze in the role that phoresis plays in the rectification of such model systems and the different mechanisms that lead to their propulsion. I will discuss the role that the dynamics of the embedding medium plays in the different regimes that characterize active colloids. These simple models will help to address the fundamental properties of active systems and I will discuss the generic implications that self-propulsion has in the emergence of structures in suspensions of model

self-propelled particles.
In general, the steady states that characterizes these systems require a consistent dynamic treatment. I will analyze the role that the medium in which active colloids displace has in generating correlations among active particles them.

I will consider different mechanisms, such as swimming or heterogeneous catalysis, which lead to spontaneous self-organization in the absence of external driving for a variety of active suspensions. Such a comparison will help to discern between specific ingredients and general features determining the emergent properties of active systems.

Participation:

In-Person

References:

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Poster / 1021

Asymptotic Homogenization - Modeling the charging behavior of Li-ion batteries

Author: Giuliano Lombardo[1]

Co-authors: Wang Yuanzhen [2]; Ulrich Nieken [3]

[1] *University of Stuttgart, Institute of Chemical Process Engineering*

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[3] *Institute of Chemical Process Engineering, University of Stuttgart*

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The modeling of lithium-ion cells plays an important role in the electrification of many industries, such as the automotive industry. Models with high accuracy and low computational complexity are essential for the optimization of such applications.

To achieve this, a fully homogenized macroscale (FHM) model has been proposed 1. This reduced model is based on effective mass and charge transport equations in isothermal active particles and electrolyte.
In current-limited battery operation, and thus at low C-rates, the FHM model works very well. At high C-rates, the predictions of the FHM model deviate significantly from those of the Direct Numerical Simulations (DNS). A high C-rate leads to high current densities between the active particles and the electrolyte and thus to steep concentration gradients near the interface. The resulting deviation between the inner concentration and surface concentration can no longer be covered by the homogenized value. Consequently, the FHM model is not applicable to diffusion-limited battery operation.

Therefore, we propose an extension of the FHM model based on Wang's diffusion length concept for spheres [2]. Here, the diffusion length is an additional variable that characterizes the correlation between the homogenized concentration and the surface concentration as a function of the C-rate. This extension allows to consider the diffusion limitation within the active particles, thus allowing a reliable application at higher C-rates.
The extended FHM model is validated using a direct numerical simulation (DNS) for the charge of a graphite half-cell. Despite the non-spherical properties of the graphite electrode, the diffusion length concept can be successfully applied. The concentrations and potential distributions of the FHM model are in good agreement with the DNS results.

Participation:

In-Person

References:

1 Arunachalam, H., & Onori, S. (2019). Full homogenized macroscale model and pseudo-2-dimensional model for lithium-ion battery dynamics: comparative analysis, experimental verification and sensitivity analysis. Journal of The Electrochemical Society, 166(8), A1380
https://doi.org/10.1149/2.0051908jes

[2] Wang, C. Y., Gu, W. B., & Liaw, B. Y. (1998). Micro-Macroscopic Coupled Modeling of Batteries and Fuel Cells: I. Model Development. Journal of the Electrochemical Society, 145(10), 3407.
https://doi.org/10.1149/1.1838820

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1022

Entropic origin of the deviations from Darcy's law in porous media

Authors: Andres Arango-Restrepo [1]; J. Miguel Rubi[1]

[1] *University of Barcelona*

Corresponding Authors: aarangor@unal.edu.co, mglrb2@gmail.com

Knowing how liquid matter moves through a crowded medium due to the action of a force is currently a problem of great practical importance, present in cases as diverse as the transport of particles across a cell membrane and through a porous medium. To calculate the mass flow through the system, we propose a model 1 that emulates the texture of the medium by means of entropic barriers that the particles must overcome to move. The model reproduces the velocity scaling behaviour with force found in many systems, showing how the scaling exponent depends on the microstructure of the medium and what the limit of validity of Darcy's law is. Our model offers a new perspective capable of characterising the flow of matter through the medium which may be useful in studies of nanofluids, oil recovery, soil drainage, tissue engineering and drug delivery.

Participation:

In-Person

References:

1 A. Arango-Restrepo and J. Miguel Rubi, J. Chem. Phys. 153, 034108 (2020)

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Energy Transition Focused Abstracts:

MS23 / **1023**

Ion adsorption at nanoscale interfaces out of equilibrium

Author: Fernando Bresme[1]

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Liquids under nanoconfinement and non-equilibrium conditions feature in many problems of interest in energy recovery, management of energy dissipation or liquid storage. Nanoconfinement influences the structure of liquids and their response to external fields. In this talk, I will discuss recent investigations, using non-equilibrium molecular dynamics techniques, on the coupling effects between nanoconfinement and external fields. I will illustrate these ideas with two examples: thermodiffusion of aqueous solutions in nanopores and nanotribology of room-temperature ionic liquids in slit nanopores.

Participation:

In-Person

References:

Bresme, F., Kornyshev, A. A., Perkin, S., and Urbakh, M., "Electrotunable friction with ionic liquid lubricants", Nature Materials, 21,848-858 (2022)

Di Lecce, S., Albrecht, T., and Bresme, F., "Taming the thermodiffusion of alkali halide solutions in silica nanopores", Nanoscale, 12, 23626-23635 (2020)

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Energy Transition Focused Abstracts:

Poster / **1028**

Pore-scale Modelling of Salt and Hydrate Formation During CO2 Injection

Author: Saleh Mohammadrezaei[None]

Co-authors: Rouhi Farajzadeh [1]; Vahid Niasar [2]

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As a greenhouse gas, CO2 contributes significantly to the rise in global temperatures. The concentration of CO2 in the atmosphere has increased by 45\% since the First Industrial Revolution, as a result of continuous CO2 emissions. In order to reduce artificial emissions of CO2 into the atmosphere, measures must be taken. Currently, fossil fuels still dominate the energy market, and CO2 capture and storage is considered the most feasible and effective method of reducing CO2 emissions. However, injection of CO2 into the subsurface water presents significant challenges, especially near the well bore. During CO2 injection into saline aquifers, salt precipitation near the well and the formation of hydrates near the well are two significant challenges reported in the literature. These challenges can result in injectivity loss if not mitigated.

Understanding the fundamental physics of the problem, identifying the critical physical and chemical parameters that may affect salt precipitation requires pore-scale insight. Pore scale simulations in contrast to Darcy-scale simulations require less requirements about fluid dynamics and reactions and thus they provide more detailed insights into the processes, but these models cannot simulate physically a large system due to computational limitations. The objective of this study is to develop pore-scale models for non-isothermal, multicomponent multiphase flows along with a geochemical simulator that can simulate thermodynamic conditions. This study will also provide recommendations on designing and the required time scale for laboratory experiments, such as salt precipitation and hydrate formation. It is also the objective of this study to investigate how porous media properties can be upscaled for given thermodynamic conditions based on dynamic conditions.

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In-Person

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Energy Transition Focused Abstracts:

1029

Physico-chemical variations of shale with artificial maturation

Author: Kouqi Liu [1]

[1] *Peking Unviersity*

Corresponding Author: kouqi.liu@pku.edu.cn

As a popular method to study systematic evolution of pore structures or geochemical properties of source rocks during thermal maturation, pyrolysis (either the hydrous pyrolysis or the anhydrous pyrolysis) is widely employed to simulate the oil generation process. However, the variations in mechanical properties of shale samples during the pyrolysis which plays important role in the hydraulic fracturing design which is one of the most important tools to increase the production are rarely studied. In this study, by using the multiple methods such as grid nanoindentation method with gas adsorption, organic petrology and bulk geochemical analysis, we evaluated the changes in mechanical properties of shale samples under both anhydrous pyrolysis (AHP) and hydrous pyrolysis (HP). The results showed that thermal maturity (%BRo) of the products is different under these two separate pyrolysis methods. Moreover, at the same pyrolysis temperature, mechanical parameters (i.e., Young's modulus, hardness, and fracture toughness) of the HP product were found to be smaller than those of the AHP. During the pyrolysis process (increasing the pyrolysis temperature), the reduction in the mechanical parameters (mean Young's modulus, mean hardness, and mean fracture toughness) following AHP and HP can be larger than 40%. This study shows that water plays an important role in changing the physico-chemical parameters during the process which should be considered in development plans of the formations that'd undergo in situ conversion.

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Energy Transition Focused Abstracts:

Poster / 1030

Sparsified coarse-scale operators for multiscale methods

Author: Omar Chaabi[1]

Co-author: Mohammed Saad Al Kobaisi [1]

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Generating a solution for the pressure in reservoir models with fine-scale heterogeneities, modeled at a meter scale, can be compute-intensive. Multiscale methods aim at reducing the runtime for the solution of Poisson-type equations by solving coarsened flow problems that account for fine-scale variations. To obtain a coarse-scale operator one needs to project the fine-scale operator using prolongation and restriction transfer operators. The choice of transfer operators determines the sparsity pattern and the quality of the coarse-scale operator. Multiscale restriction-smoothed basis (MsRSB) method and the classical multiscale finite volume (MSFV) method provide coarse-scale operators with MPFA-like stencils even when TPFA fine-scale operator is used at the fine level. Typically, the use of a denser MPFA operator is justified by its ability to capture tensorial permeability effects unlike TPFA or multiscale coarse-scale operators.
In this work, we show an algorithm that reduces the sparsity pattern of the coarse-scale operator for multiscale methods irrespective of the choice of prolongation and restriction operators. Once

the choice is made on the transfer operators, the algorithm sparsifies the coarse-scale operator to the desired sparsity pattern. We test the algorithm on the state-of-the-art MsRSB method to solve the elliptic pressure equation on 2D layers of the 10th SPE comparative solution project. The SPE10 problem has uniform structured grids with diagonal permeability tensor which motivated our choice of reducing the coarse operator sparsity to a TPFA-like stencil structure. Results show the potential of this approach as we were able to reduce the coarse-scale stencil size and get solutions with tolerable errors compared to the reference solution.

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Poster / 1031

Design of Functionalized Molecules and Polymers (FMP) for Improving the Containment of Subsurface CO2

Authors: Sina Omrani[1]; Vahid Niasar[1]

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The rise in greenhouse gas emissions, particularly carbon dioxide (CO_2), has become a significant environmental issue and is directly responsible for global warming and its harmful effects on the planet. Geological CO_2 storage (GCS) has emerged as a promising solution to reduce CO_2 emissions into the atmosphere. However, for GCS to be successful, long-term containment of CO_2 underground is essential. CO_2 leakage can occur through both engineered pathways, such as leaks associated with wells, and natural pathways, including caprock and geological faults. Existing materials developed to prevent CO_2 leakage have exhibited problems such as aggregation, degradation, high viscosity which limits the injectivity, and poor tolerance to temperature, pressure, and salinity. Therefore, it is crucial to identify materials that do not have these shortcomings to enhance the safety of GCS projects.

The aim of this research study is to design materials that are sensitive to CO_2 and have the ability to block leakage pathways while remaining stable under high temperatures, pressure, and salt concentrations. Another aspect of this study involves testing the rheology of the materials under different conditions that may be encountered during underground storage. To gain a deeper understanding of the behavior of these materials in porous media, numerical modeling will be conducted from both a pore and field perspective. As a reactive, multicomponent, and multiphase issue, this problem requires a comprehensive numerical approach. This research is also a collaboration between the University of Manchester and A*STAR institutition.

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Energy Transition Focused Abstracts:

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Classification, characteristics of shale reservoir and its significance based on the relationship between pore and surface: An example from the Paleogene shale, Jiyang Depression, Bohai Bay Basin, east China

Authors: Liu Shunyu[1]; Cai Jingong[2]

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The shale reservoir has more surface on account of the presence of nanopore, which is different from the conventional reservoir. The differentiation of fluid occurrence can occur due to the coexistence of pore and surface, that is the adsorbed and free state. However, as a result of unclear relation between pore and surface, the evaluation and classification of shale are limited from the perspective of the reservoir. In this paper, a suite of shale samples were collected from the Shahejie Formation in the Jiyang Depression for nitrogen gas adsorption (N2GA), high pressure mercury intrusion (HPMI) and field emission scanning electron microscopy (FE-SEM), thin sections observation. We analyzed the relation between the pore volume (PV) and the specific surface area (SSA), classified the shale reservoir on the basis of the relation furthermore and then discussed the characteristics and significance.

The results show there are various relationships between the different PV and the SSA. The micropore PV exhibits the strong positive correlation with the SSA. The mesopore and macropore PV indicate the similar and complex correlations with the SSA: There is a weak positive correlation when the SSA is less than 10 m2/g, but the correlation of macropore is worse. There is a weak negative correlation when the SSA is greater than 20 m2/g. It shows a transitional phenomenon in the range of 10 to 20 m2/g. The shale reservoir can be divided into the pore type, the surface-pore type and the surface type according to the relationships between the PV and the SSA. The pore type has the smallest SSA, the largest average pore size, is richer in mesopore and macropore and is poorer in micropore. Thus the adsorption potential or capillary pressure is weakest and the fluid exists in the pore in the form of slight multilayer adsorption and obvious capillary condensation, which shows the free state is dominant. The surface-pore type has the modest average pore size and SSA, is richer in mesopore and micropore, is poorer in macropore. The adsorption potential or capillary pressure is modest and the fluid exists both in the pore and on the surface saving as monolayer absorption, multilayer adsorption and capillary condensation which shows the coexistence of free and adsorbed state. The surface type has the smallest average pore size and the largest SSA, is richer in micropore, is poorer in mesopore and macropore. The adsorption potential or capillary pressure is strongest and the fluid tends to be adsorbed on the surface in a monolayer mainly and multilayer adsorption partly, which shows adsorbed state mainly.

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MS01 / **1037**

Insights into sandstone wettability alteration during cyclic $scCO_2$-brine injections

Author: Anna Herring[1]

Co-authors: Chenhao Sun [2]; Ryan Armstrong ; Zhe Li [3]; James McClure [4]; Mohammad Saadatfar [5]

[1] *University of Tennessee*

[2] *China University of Petroleum-Beijing*

[3] *Australian National University*

[4] *Virginia Tech*

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Capillary trapping (also known as "residual trapping") of supercritical carbon dioxide ("$scCO_2$") is a key mechanism contributing to the safety and security of geologic sequestration operations for carbon capture and storage (CCS). Recent experimental studies have suggested that cycles of $scCO_2$ and brine injections alter surfaces of sandstone grains and increase capillary trapping. We present results from two supercritical-condition core-flooding experiments aimed at pinning down specifics of the alteration mechanism. Multiple cycles of $scCO_2$ and brine injections were performed in two Bentheimer sandstone samples; pore pressure was monitored during injections via transducers, and after cessation of flooding, fluid configuration and $scCO_2$ trapping were visualized via 3D X-ray microcomputed tomography at the Australain National University's CTLab. We confirm previous results that demonstrated shifts in injection pressure and $scCO_2$ trapping behavior over multiple injection cycles, and we conduct additional analyses to discern the fluid-fluid macroscopic contact angle, interface mean and Gaussian curvatures, $scCO_2$ interfacial area, and topology of trapped $scCO_2$ ganglia. Microstructural analysis of the $scCO_2$ phase indicates increasing presence of relatively high contact angle (i.e. less water-wetting) surfaces as the experiment progresses, indicating a transition to a "patchy"mixed-wet state. We observe that this wettability alteration renders $scCO_2$ more stable in the rock pore space, increasing capillary trapping over four injection cycles. However, the effect is only evident for homogenous region of the core; in regions where capillary heterogeneity dominates, wettability alteration effects are not evident. These results support previous work demonstrating progressive shifts in fluid flow and trapping due to $scCO_2$/brine cycling, and provide new clarification as to the conditions under which this phenomenon may occur. [1,2]

Participation:

In-Person

References:

1 A.L. Herring, C. Sun, R.T. Armstrong, Z. Li, J.E. McClure, M. Saadatfar, Evolution of Bentheimer Sandstone Wettability During Cyclic scCO 2 -Brine Injections, Water Resour. Res. 57 (2021). https://doi.org/10.1029/2021WR030891. [2] A.L. Herring, C. Sun, R.T. Armstrong, M. Saadatfar, Insights into wettability alteration during cyclic scCO2-brine injections in a layered Bentheimer sandstone, Int. J. Greenh. Gas Control. 122 (2023) 103803. https://doi.org/10.1016/J.IJGGC.2022.103803.

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1038

Modelling contaminant migration from wastewater drain to subsurface media

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Several cities in developing world are facing growing problems of water scarcity and water pollution. The city environment is characterized by fast changing demography and landscape as witnessed by increasing population, urban sprawl, infrastructural growth, and mushrooming industries. A very critical issue of water pollution arises from the sprawling dwelling units and small-scale industries in various urban clusters because of improper management of sewage and industrial water. The untreated sewage and industrial waters are most often discharged into the natural drains, although such disposals are prohibited. The contaminants migrate from these wastewater drains to the subsurface media and percolates down through the variably saturated soil that leads to groundwater contamination in adjoining areas of the drain throughout its course of travel. The objective of this paper is to present a modelling framework of contaminant migration from wastewater drains to investigate how the contaminants affect the root zone soil quality and how much it poses contamination risk to groundwater system in the region. The modelling framework includes the channel flow hydraulics to simulate the flow behavior in wastewater drain under varying hydrodynamic conditions and Richards'equation to simulate the subsurface flow and advection-dispersion equation to simulate the multicomponent contaminant transport through the variably saturated porous medium. The modelling framework was applied to the Najafgarh drain which traverses through west, central and north parts of Delhi city before joining the Yamuna River at Wazirabad. The Najafgarh drain accounts about 69% of wastewater that is discharged into the river Yamuna and is the main culprit for deteriorating river water quality. The present study investigates the flow condition in drain and the behavior of contaminant migration from the drain to the subsurface stratum and examines potential risk of contamination to groundwater system. The subsurface flow and contaminant transport simulations were carried out using COMSOL Multiphysics software. The hydraulic properties of variably saturated porous medium were estimated using van Genuchten formula. The study reveals that the contamination spreading grows with the time as the drain flow is blocked due to filthy condition which provides greater retention time and increases seepage. The heavy sedimentation reduces seepage but becomes potential source of contaminant accumulation which can release miscible contaminants to migrate to shallow aquifers through the subsurface porous media. The contamination spreads more than 65% of the modelled domain in 10 years of time. The contaminant spreading is sensitive to the rainfall, lateral flows, and subsurface hydraulic and dispersion parameters. The study shows that there is a need of taking strategic measures to clean the drain

which will not help in reducing the pollutant load to river Yamuna but will also help to minimize the groundwater contamination risk and allow the drain to function like a recharging channel for the groundwater system and making adjoining areas ecologically rich.

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1039

Carbon Resilience Calibration Workflow for Production Decarbonization: A Carbonate Case

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In the path to a net-zero carbon and energy transition from fossil fuel, the world is facing a dilemma of growing global energy demand and required actions on climate-related risks. While over 80% of the current global energy needs are supplied by fossil fuels, 88% of estimated world greenhouse gas emissions is related to fossil fuels due to combustion, extraction, flaring and venting of associated gas. Furthermore, carbon intensity (CI) of upstream production, defined as Kg CO2e per barrel oil, has increased due to a growing reliance on unconventional and heavy oils and depletion trends in conventional resources, which make the energy sector the most sensitive sector impacted by an acceleration in the transition to green economy. Moreover, there is a huge gap in terms of scale and distribution of planned and ongoing carbon capture, utilization and storage (CCUS) plants and high CI regions, as most of the fossil fuel dependent countries (FFDCs) are least prepared for the energy transition in terms of exposure (hydrocarbon exports make up for GDP) and resilience (revenues from oil and gas sales not adequately managed) to carbon emissions associated with oil production. Therefore, the role of oil and gas companies on developing strategies for lower carbon technologies and applying decision-making workflows for sustainable resource management is highlighted to smooth the low-carbon transition period.
The focus of this work is on carbon resilience calibration and emissions scenario analysis in investment decisions to realize decarbonization goals through balancing short-term actions with long-term energy transition plans. The complex porous media and reservoir fluid properties of a carbonate oil and gas field with high CI and large flaring volumes is studied to analyze carbon footprint (CFP) and carbon risk associated to development and production operations such as drilling new wells, artificial lift systems (ALS) and oilfield-produced water treatments. A cash flow model for a sample CCUS project based on data-driven CI estimates and emission scenario analysis is proposed to promote carbon resilience calibration in decision-making process.

Participation:

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Poster / 1041

Deliquescence of salt nanocrystals

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Co-author: Michael Steiger

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Deliquescence is the process by which a solid picks up water vapor from the atmosphere spontaneously and forms a solution. The deliquescence of a salt crystal is characterized by the deliquescence relative humidity (DRH) of the salt. Salt nanocrystals deliquesces differently than the bulk salt crystals. It has been shown in previous study that in comparison to the DRH of the bulk NaCl crystals (75.3% RH), the DRH of NaCl confined in nanoporous silica materials decreases from 73 to 58% as the pore size decreases from 89 to 8 nm 1. Contrary to that, the DRH of levitated nano-sized NaCl crystal increases to 83% RH as the crystal size decreases to 6 nm [2,3].
The present work focuses on the deliquescence of salt crystals (NaCl and KNO3) confined in mesoporous SBA-15 and MCM-41 silicas having pores upto 3 nm. Salt-silica-composite materials were prepared by impregnating the porous materials with salt-solutions avoiding over-filling of the available pore volumes. After drying, water vapor sorption isotherms of bulk salts, unloaded porous materials and the respective salt-silica-composites were determined. The experimental results reveal that the deliquescence of salt crystals confined in pores occurs not only far below the DRH of bulk salts but also much earlier than the capillary condensation in the unloaded porous materials. Even the capillary condensation in unloaded MCM-41 silicas is significantly lower than the DRH of bulk salts. Thus, in contrast to DRH of levitated salt nanocrystals, the DRH of confined nanosized salt crystals decreases with decreasing pore size.
A thermodynamic model approach, based on the combination of an ion-interaction model, the Laplace equation and the Kelvin equation, is used to predict the deliquescence of both levitated and confined nanosized salt crystals. The calculations agree well with the experimental results and reveal that the shift in the DRH is largely the result of the curvature of the vapor–liquid interface that is formed during deliquescence 1. In contrast, the influence of Laplace pressure and size of the crystal on the solubility is small.

Participation:

In-Person

References:

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1042

Modelling Cellular Blood Flow in the Porous Intervillous Space of the Human Placenta

Authors: Qi Zhou[1]; Eleanor Doman[2]; Igor L. Chernyavsky[3]; Oliver E. Jensen[2]; Miguel O. Bernabeu[4]; Timm Krüger[1]

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Key words: biological tissue, porous media, haemodynamics, red blood cells, lattice-Boltzmann method

The human placenta is an evolving organ where the mother feeds her fetus with oxygen and nutrients through solute transport processes, which rely on robust maternal blood flow in the highly heterogeneous intervillous space (IVS) resembling random porous media in nature [1,2]. Since flow channels within the IVS are sometimes comparable in size with red blood cells (RBCs), the cellular character of blood can lead to rheological behaviour that existing continuum models fail to capture [3]. In this work, we consider blood as a suspension of deformable RBCs in plasma and model cellular blood flow across realistic IVS domains, to enable a mechanistic understanding of the structure-function relationship between the IVS's architecture and haemodynamics.

First, 3D IVS domains were reconstructed from synchrotron micro-CT image stacks of the human placenta tissue (Fig. 1a) [4]. Cellular blood flow of designated feeding haematocrits (i.e. HF, volume fraction of RBCs) in the reconstructed flow domain was then simulated with our high-performance parallel blood flow simulator HemeLB (open source: https://github.com/hemelb-codes/hemelb) using the lattice-Boltzmann and immersed-boundary methods [5]. For comparison, homogeneous Newtonian flow with physiological blood viscosity and pure plasma flow with liquid water viscosity were also simulated.

Our preliminary flow simulations in a large IVS domain (Fig. 1a) recapitulate the exponential flow distribution reported for IVS flow [4], either for homogeneous blood or for dilute RBC suspension (HF = 1%). Further simulations with homogeneous blood along three principal directions of a cropped cubic domain (Fig. 1b) reveal a moderate degree of flow anisotropy. For semi-dilute RBC suspension (HF = 10%, Fig. 1c), the flow resistance in the three directions varies as evaluated by the apparent viscosity of the suspension relative to plasma viscosity, although the RBC residence time

distributions are similar (Fig. 1d). The RBC deformability is also found to have a notable effect, with elevated viscosity for hardened cells. These cell-scale haemodynamics investigated in our work can help elucidate the elusive structure and function relationship in the IVS which may explain how impaired placenta architecture causes pregnancy pathologies.

Participation:

Online

References:

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Poster / 1043

Study on the Law of CO2 Miscible Displacement Under Different Injection Methods in Heterogeneous Reservoir

Authors: Xinliang Chen[1]; Yu Hongwei[2]; Zhengming Yang[2]; Wen Li[1]; Meng Du[1]; Zhongkun Niu[1]; Yilin Chang[1]

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Abstract: There is still more residual oil in heterogeneous reservoirs after water injection, and it is difficult to recover them by further water flooding. As a common gas flooding medium, CO₂ can further improve the recovery of heterogeneous reservoirs after water flooding, so it is of great significance to study the laws of CO₂ miscible flooding under different injection methods in heterogeneous reservoirs. In this study, according to the heterogeneity characteristics of Lunnan Oilfield in Tarim, China, a single 1 m double-layer long core model was designed and prepared, and CO₂ miscible displacement experiments with four different injection methods were carried out. Through the comparison and analysis of the experimental data, the displacement effect of CO₂ miscible flooding under different displacement methods is obtained, and the laws of CO₂ miscible flooding under different injection methods in heterogeneous reservoirs are summarized. The research shows that: ① The oil displacement efficiency of different injection methods of CO₂ miscible flooding in heterogeneous reservoirs from high to low is: CO₂-water alternate injection, continuous CO₂ flooding, periodic CO₂ flooding, and CO₂-hydrocarbon gas alternate injection. ② CO₂ miscible flooding in heterogeneous reservoirs mainly relies on convective diffusion and miscible mass transfer to recover crude oil. ③ The effect of convective diffusion mainly depends on the plugging of the dominant channels in high-permeability areas and the control of injection-production pressure differential. The effect of miscible mass transfer mainly

depends on the degree of displacement in the early stage and the strength of gas miscibility. ④ To improve the recovery efficiency of CO₂ miscible flooding in heterogeneous reservoirs, on the one hand, gas channeling should be slowed down, dominant channels should be blocked, and displacement pressure differential should be improved. On the other hand, the miscibility of CO₂ should be improved.
Keywords: Different injection methods; Heterogeneous reservoir; CO₂ miscible flooding;

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Energy Transition Focused Abstracts:

1044

Porous biohybrid multifunctional membranes for biosensors and bioremediation

Authors: Lidietta Giorno[1]; Fabio Bazzarelli[None]; Rosalinda Mazzei[None]; Emma Piacentini[None]; Teresa Poerio[None]; Serena Regina[None]; Giuseppe Vitola[None]

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Synthetic membranes are among the most effective technology in separation, fractionation, concentration, and purification. Their nanostructured pores have demonstrated their unique role also in implementing processes such as catalysis, and molecular recognition. Engineering the chemistry of the material, the structure of the pores, and the process conditions permits an extension of the areas of application of membranes. The combination of porous and mesoporous membranes with biomolecules leads to the development of artificial membranes with biofunctional properties. Biorecognition and bioconversion confined in micro and nanoscale compartments are emerging as important properties in the development of membrane-based biosensing and biocatalytic tools. For example, the trace presence of recalcitrant micropollutants (such as pesticides, antibiotics, hormones, etc.) in the environment causes chronic exposure that represents a threat to health and socio-economic wellness. The availability of technologies able to detect and eliminate trace micropollutants appears to be crucial.
The lecture will discuss the development of biofunctionalized porous membranes and their ability in intercepting traces of a model pesticide (such as paraoxon). The capability of membranes functionalized with an enzyme (phosphotriesterase) to fully degrade the pesticide will be also illustrated.
Superparamagnetic plasmonic nanoparticles (core-shell iron-gold nanoparticles) conjugated with enzymes are orderly arranged in porous polymeric frameworks able to accumulate the trace contaminant and enhance the interaction with the biochemical receptor. The role of membrane material, pore size, structure, morphology, topography, thickness, and surface energy on the mass transport, molecular interaction, and stabilization of the biomolecules will be outlined.

Participation:

In-Person

References:

The authors would like to thank POR Calabria FESR-FSE 2014/2020 for the financial support to the SmartMatter project within the M-ERA.NET Call 2019.
National Research Council of Italy, Institute on Membrane Technology, CNR-ITM, Via P. Bucci, 17C, 87036 Rende (CS), Italy

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Poster / 1045

A visualization study of stress evolution in CBM horizontal well cavity completion

Authors: Xiaozhou Qin[1]; Ruiyue Yang[1]; Zhongwei Huang[1]; Jianxiang Chen[1]; Meiyang Jing[1]; Jiawen Li[1]

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The efficient exploitation of coalbed methane (CBM) plays an important role in reducing outburst hazards, securing energy supply and reducing carbon footprint. Horizontal well cavity completion performs well in Zhengzhuang Block, China, with stable daily gas production of 10,000 m3, which was four times more than that of the adjacent fractured well. However, the stimulation mechanism of horizontal well cavity completion is not clear and it is a challenge to directly reveal the evolution of stress and strain. This study proposes a method, finite discrete element method (FDEM), for characterizing fracture and describing stress and strain evolution. A visualization experimental device based on digital image correlation (DIC) was proposed to measure the strain field. Then the established FDEM model is calibrated based on observations from the experiment. And the effects of cavity diameter and in-situ stress on short-term response of stress evolution and fracture extension were investigated. The results show that numerical simulations are in good agreement with the experimental observations. The stress concentration occurs first around the cavity, and then induces fracture propagation, which further leads to stress release. The fracture extension and stress relief is limited in the vertical direction as the vertical stress decrease. The fracture length grows linearly with cavity diameter. The key findings of this study provide insights into the progress of stress reconstruction and fracture extension in CBM horizontal well cavity completion.

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Poster / 1046

Experimental Study on Stress Sensitivity Considering Different Fractures and Water Content in Shale Reservoir

Authors: Jin Chang[1]; Zhiming Hu[1]; Xianggang Duan[1]; Yuanyuan Li[1]; Ke Xu[1]

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Large-scale fracture network and fracturing fluid retention in shale reservoir will inevitably affect the stress sensitivity. We focused on different areas of shale gas flow, and design several stress sensitivity tests of matrix, unsupported fracture, supported fracture and water-bearing fracture cores. The influence of different types of fractures and fracture water content on permeability is clarified. Further more, a characterization model describing the change of permeability with stress is established. The result shows: The stress sensitivity of different areas varies greatly. The loss of conductivity of support fracture is small under high stress conditions. But the loss rate of unsupported fracture permeability under the effect of effective stress is up to 97%, and the permeability recovery rate after stress recovery is less than 20%. Permeability decreases by 3-4 orders of magnitude after microfracture water cut, which is more sensitive to stress change. The research support the optimization of fluid filling intensity and flowback system of shale gas wells.

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Energy Transition Focused Abstracts:

Poster / 1047

A process-based approach to study the effect of microporosity on flow properties in carbonate rock

Authors: Anup Shahi [1]; Kumar Hemant Singh[2]; Ranjith PG[3]

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Carbonate rocks are highly heterogeneous due to post-deposition physical and chemical changes. It exhibits various types of pores and a wide range of pore size distribution, making it challenging to capture all pores in a single pore geometry model obtained from imaging techniques used in Digital Rock Physics (DRP).
Digital rock analysis has proven to be promising and time efficient in deriving the pore-scale perspective of reservoir rock using simulation based on 2D or 3D image data. 3D models of rock microstructures are required to predict the rock properties without performing lab experiments; however, in the case of carbonate, DRP is affected by a trade-off between image resolution and Field of view.
Here we are presenting a process-based approach to creating 3D pore geometry of carbonate rock which incorporate micro and macro pore in the 3D geometry. The developed 3D model was used to study the effect of microporosity on rock permeability and elastic properties.
In the present study, SEM images, thin sections, and XRD data are analysed for the size and shape of pores, pore geometry, mineral composition, and diagenesis process.
Two 3D digital samples of highly heterogeneous carbonate rock, one with micro porosity and the other without micro pores, were synthetically created based on the input of pore characteristics, mineral content, and diagenesis. The pore scale simulation was performed on synthetic 3D geometry using the Finite volume method and Pore Network modelling.
In parallel, we have scanned an actual sample at two scales (high and low resolution), we used the extracted pore network information from two data sets to create a single pore network stochastically.
The results from the process-based and stochastical pore networks were compared and analysed for their efficiency in predicting the rock properties. We have also compared our results with experimental data, which is in good agreement.

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1048

Understanding the impacts of heat losses on applied smouldering systems

Author: Tarek Rashwan[1]

Co-authors: Marco Zanoni [2]; Taryn Fournie [2]; Seyed Ziaedin Miry [2]; Jiahao Wang [2]; Gavin Grant [3]; Jose Torero [4]; Jason Gerhard [2]

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Applied smouldering systems harness waste combustion within porous media to drive thermally efficient environmental engineering processes. These systems use various reactor orientations for a range or purposes, like (i) hazardous liquid management, (ii) faeces management in off-grid latrines, (iii) wastewater sewage sludge treatment, (iv) waste-to-energy, and (v) resource recovery. These systems provide unique benefits over other thermal treatment systems due to their broad operational limits offered by smouldering's inherently resilient combustion characteristics. Practically, this means that smouldering systems can manage traditionally problematic waste streams with minimal energy input, e.g., those with low-volatilities and high moisture contents. Smouldering is driven by coupling heat and mass transfer within porous media with chemical reactions. These combined processes lead to a series of distinct smouldering zones characterized by their dominant process, i.e., the cooling zone, reaction zone, and preheating zone. Ultimately, the rate of smouldering is limited by oxygen diffusion in the pore space to the fuel surface, which leads to characteristically cool peak temperatures, slow propagation velocities, and gradual heating rates. These characteristics foster a highly energy-efficient thermal treatment process.

Engineers and researchers are making strong progress in better understanding and unlocking the potential of these systems across scales. However, the impacts of heat losses on applied smouldering have not been rigorously investigated. This research gap inhibits the design and progress in applied smouldering systems development.

This presentation presents the culmination of seven years in experimental work and analyses to better understand the effects of heat losses in these systems. This work led to valuable insights into the impacts of heat losses on applied smouldering systems. These insights clarify various key phenomena, such as: (i) the key sensitivities in the global energy balance to system scale, (iii) the impacts of non-uniform air flux due to heat losses, and (iv) the steady-state behaviour in smouldering systems when the rate of global losses balance the energy released from smouldering. Altogether, these insights shed light on many multidimensional phenomena in smouldering systems due to heat losses and tool engineers to design improved applied smouldering systems for various environmentally-beneficial purposes.

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Energy Transition Focused Abstracts:

Poster / 1049

Understanding Pore Connectivity in Hard-Templated Carbon Materials

Author: Nicola Michel Seraphim[None]

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Following the need for clean energy transit and lowering carbon emissions, many electrochemical devices have been put out as energy storage tools such as fuel cells, batteries, supercapacitors, etc. all these applications require electrodes with high surface area, good flow, and mass transport hosts active material and releases bubbles. For these properties, we introduce porosity into our electrodes. However, what is important in porosity, how can we control it, and which properties are critical for catalytic purposes?
Pore Connectivity is a critical aspect in templated carbons that is usually dismissed or overdone, adding more template and connecting the nodes in the system shows percolation behavior in porosity, as properties grow after the percolation threshold where connectivity is satisfied. In this work, we analyzed two carbons (PAN and glucose) produced through a hard template synthesis (zinc oxide and silica) with a changing template ratio to understand the way the pore architecture is molded and formed. Using N2 BET adsorption, Computational simulations, and different electrochemical measurements. we report the findings that porosity produced via hard templated carbons behaves as a step function and so do many other properties which are derived from the surface area change. We observed many properties of these hard-templated carbons acting as a percolation phenomenon (step function behavior). For ZnO templated PAN carbons plotting the SSA and ECSA as a function of template ratio generated a percolation (step-function) type behavior, this was also seen in other measurements with, RDE measurements, as well as computational calculation of the surface area producing the same phenomenon and confirming even further the percolation effect in connectivity.

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Energy Transition Focused Abstracts:

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Optimization of porous structures for efficient heating/cooling

Author: Natalya Kizilova[1]

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Most flow-based domestic and industrial heaters/coolers are composed as a set of plates, tubes and/or fins with certain constant temperature kept at the solid surfaces. The problem of their design optimization aimed at faster heating/cooling of the higher volumes of fluid per unit time with lower

energy costs is very important for all types of thermomechanical units from macro to micro and nanofluidic systems. In this study the regular and fractal type porous structures are studied as optimal nature inspired design taken from nasal ducts of Arctic seals 1. Their nasal cavity can be modeled as a circular tube with a porous structure inside that is used for splitting of the flow into small jets which are in direct contact with the heating/cooling walls. Constant temperature $T_w = T* = const$(i), heat flux $J_w = const$ (ii) or convection $J_w = -\lambda\left(T - T*\right)$(iii) boundary conditions (BC) at the solid walls can be used for different types of heaters/coolers.

A regular-type porous model as a set of parallel channels with circular, square and triangle cross-sections is considered. In the steady fluid flow case $Q = const$, analytical expressions for the pressure $P\left(\vec{r}\right)$, temperature $T\left(\vec{r}\right)$ and flow velocity $\vec{v}\left(\vec{r}\right)$ are known with BC (i),(ii),(iii). As optimization criteria the hydraulic resistivity $Z_{hydr} = \left(P_{in} - P_{out}\right)/Q$, thermal resistivity $Z_{th} = \left(T_0 - T*\right)/J_{th}$, inlet length L_{in}(Fig.1b), and entropy production in the irreversible processes [2] $\dot{S}_{irr} = \int\limits_V \left(\frac{\lambda}{T^2}\left(\nabla T\right)^2 + \frac{\Pi:\nabla v}{T}\right)dV$, where Π is the viscous dissipation have been considered. The problem $\{F_j \to min, V_s = const\}$, where $\{F_j\}_{j=1}^4 \in \left(Z_{hydr}, Z_{th}, L_{in}, \dot{S}_{irr}\right)$ and V_s is the volume of solid material in the system, has been solved based on the analytical expressions.

It was shown, different sets $\{a, b, H, W, L\}$are produced by $Z_{hydr} \to min$ and $Z_{th} \to min$criteria. Optimal solutions have been proposed base on the Pareto frontiers (Z_{hydr}, Z_{th}) and (Z_{hydr}, L_{in}). Analytical solutions have been checked by CFD computations. It was shown, the approach $\dot{S}_{irr} \to min$ produce unambiguous and more efficient design accounted both viscous and thermal energy loss.

Participation:

Online

References:

1 Flekkøy, E. G., L. P. Folkow, S. Kjelstrup, M. J. Mason, and Ø. Wilhelmsen, 2023. Thermal modeling of the respiratory turbinates in arctic and subtropical seals. J. Thermal Biol. 103402. doi: 10.1016/j.jtherbio.2022.103402
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Energy Transition Focused Abstracts:

Poster / 1051

Sound and x-ray vision of a porous rock: micromechanics of shear failure under different loading protocols and implications for managing induced seismicity during subsurface operations

Authors: Alexis Cartwright-Taylor[1]; Maria-Daphne Mangriotis[2]; Ian G. Main[2]; Ian B. Butler[2]; Florian Fusseis[2]; Andrew Curtis[2]; Andrew F. Bell[2]; Martin Ling[3]; Edward Andò[4]

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Progress towards a net zero carbon economy involves subsurface activities, such as geothermal energy production and geological storage of carbon dioxide, hydrogen and radioactive waste, that disturb tectonic stresses in the Earth's crust. Seismicity induced by such stress perturbations is associated with risk from damage due to ground motion, fluid leakage and pollution due to increased permeability, and the potential loss of public confidence. Safe operation of these activities therefore requires effective management to minimise induced seismicity. Failure in brittle, porous materials initiates when structural damage, in the form of smaller-scale fractures, localises along an emergent failure plane or 'fault' in a transition from stable crack growth to dynamic rupture. Due to the extremely rapid nature of this critical transition, the precise micro-mechanisms involved are poorly understood and difficult to capture. However, these mechanisms are crucial drivers for earthquakes, including induced seismicity, and other devastating phenomena.

Here we observe these micro-mechanisms directly by controlling the rate of micro-seismic events to slow down the transition in a unique triaxial deformation apparatus that combines acoustic monitoring with contemporaneous in-situ x-ray imaging of the microstructure. We compare the seismic signatures from this experiment with those from a sister experiment carried out under constant strain rate loading. The results [1, 2] provide the first integrated picture of how damage and associated micro-seismic events emerge and evolve together during localisation and failure and allow us to directly constrain the partition between seismic and aseismic deformation at the micro-scale.

The evolving damage imaged in the 3D x-ray volumes and local strain fields undergoes a breakdown sequence involving several stages: (i) self-organised exploration of candidate shear zones close to peak stress, (ii) spontaneous tensile failure of individual grains due to point loading and pore-emanating fractures within an emergent and localised shear zone, validating many inferences from acoustic emissions monitoring, (iii) formation of a proto-cataclasite due to grain rotation and fragmentation, highlighting both the control of grain size on failure and the relative importance of aseismic mechanisms such as crack rotation in accommodating bulk shear deformation. Dilation and shear strain remain strongly correlated both spatially and temporally throughout sample weakening, confirming the existence of a cohesive zone, but with crack damage distributed throughout the shear zone rather than concentrated solely in a breakdown zone at the propagating front of a discontinuity.

Contrary to common assumption, we find seismic amplitude is not correlated with local imaged strain. The seismic strain partition coefficient is very low overall and locally highly variable. Local strain is therefore predominantly aseismic, explained in part by grain/crack rotation along the emergent shear zone. Reactive loading to maintain a constant micro-seismic event rate increases the seismic b-value, decreases the maximum event magnitude, and reduces the seismic strain partition coefficient compared with loading under a constant strain rate. Adding event rate control to that of maximum recorded magnitude may therefore be more effective than the current 'traffic light' system (based on maximum magnitude alone) for managing the risk of induced seismicity.

Participation:

In-Person

References:

1 Cartwright-Taylor et al. (2022), Seismic events miss important kinematically governed grain scale mechanisms during shear failure of porous rock, Nature Communications 13, 6169. https://doi.org/10.1038/s41467-022-33855-z.

[2] Mangriotis et al. (in prep), Micromechanics of failure in a sandstone: loading controls on seismic signatures.

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Energy Transition Focused Abstracts:

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Poster / 1052

Drag Reducing Agents for Geothermal Applications

Author: Sian Jones[1]

Co-authors: Ronald Driessen [2]; Dries van Nimwegen [2]; Pejman Shoeibi Omrani [2]; Pacelli Zitha [1]

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[2] *TNO*

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Drag reducing agents (DRAs) are molecules that are able to reduce the frictional losses in turbulent flows. Typical examples are high molecular weight polymers, or surfactants that form worm-like micelles. DRAs are widely used in industrial applications : for example they can be used to reduce the pumping requirements in long pipelines such as the Trans-Alaska pipeline (1), to increase the flow rate in fire-fighting systems (2), and to reduce operating costs in district heating networks (3). The aim of the current work is to assess the viability of DRAs for geothermal energy systems, with the aim of reducing the pumping costs at both the production and injection wells. In particular, we want to know how these DRAs interact with the subsurface. For example, the DRAs being tested might have the ability to significantly reduce drag, but this benefit would be negated if they are then shown to cause injectivity problems in the reservoir.

In this work, a number of potential DRAs, both polymers and surfactants, were obtained and two sets of screening tests were carried out to identify the strongest candidates. Firstly, the DRAs were tested for their thermal stability at reservoir salinities and temperatures. Several of the DRAs showed precipitation and phase separation at the test conditions, and were therefor removed from the study. Secondly, high-shear rheometric tests were performed with the DRAs to determine if they can provide drag reduction in turbulent Couette flow. These tests allowed us to determine the optimal concentrations for each DRA, and how this optimal concentration varies as a function of temperature.

Following these screening tests, the most effective DRAs were flowed through natural porous media samples (Bentheimer sandstone) to test for injectivity problems. It was found that for slow flows, i.e. a low shear state, there was little injectivity decline, whereas for strong flows, significant injectivity decline could be seen at the inlet of the porous media for some of the DRA samples.

Finally, in ongoing work, the final candidate DRAs will be tested in a large scale flow-loop to confirm the scale of the drag reduction that could be observed in pipe flow. A preliminary flow-loop test has been carried out with a DRA from literature (4), and drag reduction of up to 75% was observed.

Participation:

In-Person

References:

1 E. D.Burger et al. (1980). Studies of Drag Reduction Conducted over a Broad Range of Pipeline Conditions when Flowing Prudhoe Bay Crude Oil. doi.org/10.1122/1.549579
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3 A. Krope et al. (2010). Drag reducing surfactants for district heating. doi.org/10.1016/j.applthermaleng.2009.12.012
4 R.J.A. Driessen (2022). Scaling rules for DRAs in turbulent pipe flows. Internship report, TNO.

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Energy Transition Focused Abstracts:

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Poster / 1055

Predicting the heat depletion characteristics of hydrothermal doublet systems under varying reservoir and operational conditions

Authors: C. Justin Ezekiel[None]; Anozie Ebigbo[1]; Thomas Finkbeiner[2]; P. Martin Mai[None]

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[2] *Kaust*

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Geothermal power output and the associated heat depletion in hydrothermal doublet systems depend largely on the existing reservoir and operational conditions. In this study, we use CMG-STARS Simulator to numerically simulate the temperature depletion of a homogeneous, horizontal hydrothermal reservoir in Western Saudi Arabia due to geothermal exploitation by a well doublet. We vary the reservoir, operational, and boundary conditions to account for uncertainty or natural variability in the model and to calculate the corresponding variations in thermal power generation over time. For a given reservoir depth, thickness, pressure-and-temperature-related parameters, permeability, flow rate, and well configuration, it is imperative to determine the optimal well spacing to achieve the largest thermal energy generation over the lifetime of the hydrothermal reservoir. To determine the optimal doublet spacing would require hundreds, if not thousands, of permutations of the different uncertain or naturally variable reservoir and operational parameters for any specific hydrothermal system. In this study, we develop a novel generalized non-dimensional expression of power generation over production time. The dimensionless power is calculated as the ratio of the enthalpy difference between the geofluid at the production wellhead and at the injection wellhead to the enthalpy difference between the geofluid at the initial reservoir condition and at the injection wellhead. A dimensionless time is also calculated as a function of circulation flow rate, fluid density, porosity, doublet spacing, reservoir thickness, and time. We conducted simulations varying these parameters. The results tend to collapse onto a single curve in this non-dimensional phase diagram. Hence, this graphical representation can be used to predict the evolution of power over time for various combinations of the parameters without running new simulations. From this dimensionless power-time plot, the thermal power output can be calculated at four critical dimensionless times, which include the power output at (i) $\tau_d=0$ (start of production), (ii) $\tau_{d,max}$ signifying the dimensionless time at maximum thermal power output, (iii) the dimensionless thermal breakthrough time, $\tau_{d,TB}$. With this value, the thermal breakthrough time of a doublet for the hydrothermal system considered in this study can be determined without carrying out computationally expensive simulations. Lastly, (iv) dimensionless time after the thermal breakthrough has occurred, $\tau_d>\tau_{d,TB}$. The heat depletion at this stage can be expressed mathematically as an exponential decay.
Hence, for any combination of the reservoir and operational parameters, the optimal well spacing that provides the largest thermal power output over the reservoir lifetime and what combination of the parameters depletes the reservoir heat the fastest can be provided easily with the dimensionless power-time plot.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

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Poster / 1056

Comparing 2D micromodel patterns for pore-scale Underground Storage studies

Authors: Alice Massimiani[1]; Panini Filippo[1]; Dario Viberti[1]; Simone Luigi Marasso[1]

Co-authors: Nicolò Vasile [1]; Quaglio Marzia [1]; Christian Coti [2]; Donatella Barbieri [2]; Francesca Verga [1]; Pirri Fabrizio [1]

[1] *Politecnico di Torino*

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Among the strategies that are being undertaken to decarbonize the energy sector, many options involve underground hydrogen and carbon dioxide storage facilities. Therefore, efforts are being addressed to understand and characterize flow phenomena occurring in underground porous systems.

In this context, microfluidics offers a cost-effective option to extract large sets of information at the pore-scale. Microfluidics makes it possible to perform a wide series of experiments, having full control over the porous system and the experimental conditions, with little consumption of materials and fluids. Although microfluidic works on pore-scale analysis for underground fluid storage can already be found in literature, to the best of our knowledge a comparison between different porous patterns within the same experimental conditions is still missing.

In this work, we design, characterize, and fabricate four different micromodels, and we perform cycles of air/water drainage and imbibition, at different capillary numbers, to observe the influence of the network geometry on the fluid dynamics.

The four micromodel patterns respectively represent a regular grid, a Voronoi diagram, a mosaic composed of repeated images extracted from real Hostun rock thin sections, and a synthetic anisotropic porous medium generated with the QSGS algorithm. The design of these porous networks follows an increased level of complexity. All these patterns are fully characterized in terms of porosity, tortuosity, and pore size distribution using a methodology based on the A* algorithm and CFD simulation. Air/water drainage and imbibition tests are performed at standard conditions.

With this approach, we create a set of pore-scale observations that are meaningful for further understanding and future modeling of underground fluid storage sites. In particular, we describe and

compare the pore-scale phenomena and percolation patterns observed in the four micromodels, under the same experimental conditions. The strengths and limitations of 2D microdevices applied to the study of underground porous systems are discussed with respect to the observed results.

Participation:

In-Person

References:

Massimiani, A.; Panini, F.; Marasso, S.L.; Vasile, N.; Quaglio, M.; Coti, C.; Barbieri, D.; Verga, F.; Pirri, C.F.; Viberti, D. Design, Fabrication, and Experimental Validation of Microfluidic Devices for the Investigation of Pore-Scale
Phenomena in Underground Gas Storage Systems. Micromachines 2023, 14, 308. https://doi.org/10.3390/mi14020308

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Energy Transition Focused Abstracts:

MS11 / 1057

Measurement of surface charge at immiscible liquid-liquid interface using streaming-potential-on-microfluidics

Authors: Yunfan Huang[None]; Amer Alizadeh[None]; Fanli Liu[1]; Moran Wang[1]

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Surface charging at immiscible liquid-liquid interface is essential to the emulsion stability, surfactant adsorption, and various engineering applications such as drug delivery and mineral flotation. However, droplet electrophoresis, as a widely-used electrokinetic method to measure the surface charge density, has various limitations in physical modeling and sample preparation. In this work, an alternative experimental method based on streaming potential setup is proposed. A Y-Y shaped microchannel was used to make a flat and stable liquid-liquid interface. The inner wall was coated with polymer to suppress the interference of the solid-liquid interfacial electrokinetics in the liquid-liquid one. The experimental setup was first verified by revisiting the aqueous solution-silicon surface charging, after which the surfactant-free decane-KCl solution interface charging was investigated. The negative surface charge at the decane-KCl solution interface is confirmed and is found to increase when increasing the pH. This result is compatible with the probable charging mechanism that the acquired negative surface charge results from hydroxyl ion adsorption onto the interface. The proposed method enables the simplicity and flexibility for further side-by-side studies on the liquid-liquid interface charging mechanism and will inspire the quantitative macroscopic interfacial modeling for numerous scenarios, such as the droplet electrophoresis and interfacial electrohydrodynamics.

Participation:

In-Person

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Energy Transition Focused Abstracts:

1058

Indoor Physical Model Experiment Study on the Influence of Intra-layer and Inter-layer Turbulent Flow on the Sweep Volume

Authors: Xiaofeng Zhou[1]; Fahimeh Hadavimoghaddam[1]; Abdumalik Gayubov[1]; Xiao Zhang[2]; Abdulrahman Ali Almalki[3]; Alexei Rozhenko [4]

[1] *Key Laboratory of Continental Shale Hydrocarbon Accumulation and Efficient Development (Northeast Petroleum University), Ministry of Education, Northeast Petroleum University*

[2] *School of Petroleum Engineering, Northeast Petroleum University*

[3] *King Saud University*

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The prospect of finding new fields for oil and gas-based energy sources faces critical challenges. These challenges can be successfully addressed through enhanced oil recovery. Water cut, production costs, and oil recovery are all adversely affected by premature water channeling. Increasing heterogeneity in oil fields has led to the use of more and more profile control techniques. Polymer flooding has been widely used and recognized for its low cost and ease of use.

In this study, a series of flat core models including a water injection well and four production wells, each with different thickness and heterogeneous zone electrodes, have been developed using the parameters of reservoir permeability (200/400/600mD) and reservoir thickness ratio (3:3:4) of Sa II of Beierxi. In heterogeneous flat plate rock core models, electrodes are placed at the top of the medium and low permeability reservoir to improve saturation measurement accuracy. Using comprehensive analysis, the experimental results of the schemes are compared, and corresponding conclusions are drawn.

Using actual injection parameters in the field, we designed four types of flooding experiments in flat cores using different injection-production cycles. With different water permeability values, we tested a series of standard curves corresponding to resistance and oil saturation. Different resistance values can directly reflect different oil saturation values in the core since other components are not conductive. The displacement effect and swept volume after pressure system changes are clarified by using the electrode plate core as a physical model experiment. Compared with conventional water injection, cyclic water injection can further expand the swept volume of medium and low permeability reservoirs with dominant flow channels, and improve the producing degree of the top and middle layers of thick oil layers, and cyclic water injection increases the average recovery percent of reserves up to 1.04 % in thick oil layers.

In an experiment involving constant pressure water injection, the recovery percent of high, medium, and low reservoirs increased by 3.83%, 1.74%, and 1.01%, respectively, and total recovery percent increased by 2.25% with an increase in injection pressure (from 0.16 MPa to 0.20 MPa).

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Energy Transition Focused Abstracts:

Poster / 1059

A combined experimental and modeling study to evaluate the soil-gas monitoring for early detection of contaminants leakage into groundwater

Authors: Dorian Davarzani[1]; Amir Alamooti[1]; Nicolas Aubert[1]; Daniel Hubé[1]; Valérie Guérin[1]; Marc Crampon [1]

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Groundwater monitoring is the most widely used technique to detect non-aqueous phase liquid (NAPL) leakage from underground storage tanks. However, this method allows the detection of leakage as soon as the pollutants reach the groundwater table, dissolve, and move forward to the monitoring wells. In addition, this technique is often expensive and has to be accurate enough to allow rapid identification of the source in case of sudden detection of pollutants. Here, we present a new detection method for the leakage of volatile compounds in the soil before reaching the groundwater by monitoring the soil gas. A model has been developed to validate the proposed monitoring technique by the NAPL leakage from an underground reservoir tank. The model simulates the pollutant infiltration into the unsaturated porous media using the generalized Darcy's equations and the soil gas extraction using the advection-diffusion equation, taking into account the gas adsorption onto grain surfaces. A decimetric-scale 2D tank experimental setup filled with different sand sizes was used to validate the developed model. The front part of the 2D tank was made of transparent glass to photograph the NAPL front propagation using the light-reflected method. We investigated the infiltration of two light NAPLs (diesel fuel and gasoline) from the middle top of the tank and different gas extraction flow rates. The gas extraction was performed from a port on the middle right side of the tank. The extracted gas was analyzed continuously using a portable gas chromatograph. The comparison of experimental and numerical results for LNAPL front propagation and gas concentration allowed the validation of the developed model. Therefore, the impact of the soil gas monitoring well distance from the leakage source, extraction flow rate, and soil and pollutant type on detection efficiency have been tested using the numerical model at a real scale. The results demonstrated that the proposed soil gas monitoring technique could detect pollution with a low soil-gas extraction flow rate in a radius of tens of meters around the soil gas monitoring well and after a few months for high and medium soil permeability.

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In-Person

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Energy Transition Focused Abstracts:

Poster / 1060

On the use of tortuosity for modelling Li-ion battery separators

Authors: Isaac Paten[1]; Martin Petitfrere[2]; Olivier Liot[3]; Céline Merlet[4]; Romain De Loubens[2]; Michel Quintard[1]; Yohan Davit[1]

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Currently, the industry standard for modelling Li-ion batteries at cell scale is known as "Porous Electrode Theory."This approach has prevailed for about 50 years, and still undergirds the majority of commercial software and academic tools for this application. The macroscale equations employed in these models typically use a single tortuosity factor to estimate both effective diffusivity and ionic conductivity. Furthermore, it is standard practice to use the Bruggeman correlation to calculate this tortuosity factor, despite its validity for this application being the subject of some dispute 1. In recent years, various authors have explored the versatility of the Bruggeman correlation for Li-ion battery electrodes [2, 3], but there has been comparatively little investigation of the battery separator. In this work, the pore-scale transport equations are upscaled using a volume-averaging method, giving insight into the possible structure of the macro-scale equations, and the nature of the effective properties, thus highlighting which assumptions are implicit in the use of a single tortuosity factor. Additionally, effective transport properties for a Celgard® PP1615 battery separator are derived directly from tomographic images, to evaluate if the Bruggeman correlation is appropriate, and to further clarify if using a single tortuosity factor is reasonable. To do so, concentrated-solution transport equations are solved over a reconstruction of the separator geometry whilst imposing various Dirichlet conditions on electrolyte concentration and potential. To give a benchmark for comparison, the pore-scale transport equations are solved for a separator sample under realistic discharge conditions, allowing evaluation of the accuracy gain offered by a macroscale model with tomography-derived transport properties.

Participation:

In-Person

References:

1 Tjaden, B., Cooper, S. B., Brett, D. J. L., Kramer, D., & Shearing, P. R. , Curr. Opin. Chem. Eng. 12 (2016), 44–51.
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Poster / 1062

CO2 Fluid Properties Parametrization for Accurate Heat, Solubility and Transport Model

Authors: Bora Yalcin[1]; Justin Ezekiel[1]; P. Martin Mai[1]

[1] *KAUST*

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As an alternative to water, supercritical carbon dioxide (CO2) has higher mobility and heat capacity to be used for heat extraction from geothermal reservoirs, while also trapping most of the injected CO2 underground to reduce carbon emissions and mitigate climate change. CO2 capture, utilization, and storage (CCUS) in geothermal reservoirs has become an attractive option for circular carbon economy models for governments and green energy business decision takers. Therefore precise fluid property parametrization and modeling workflows are essential for CCUS simulations to reach the right economic decisions.

CO2 injection in a saline aquifer is a multi-phase flow problem where scientists have to take into account the multi-component fluid flow and heat transport. For many multi-phase flow systems, viscosity plays an important role; hence it characterizes the fluids' resistance to flow (mobility) and the displacement rate of other fluids in the reservoir. In cases of injecting CO2 in thick, deep, saline aquifers, where the changes in pressure and temperature are considerably high, the viscosity of the injected fluid is also changing significantly in reservoir conditions. Moreover, the mutual solubility of CO2 and water has many obvious implications for long-term carbon sequestration and fluid-rock-heat interactions, which also changes with pressure and temperature. Therefore fluid properties, especially the viscosity and solubility of CO2, is critical to be prescribed precisely in the expected ranges of pressure and temperature of reservoir conditions.

We prescribed the CO2 viscosity based on the National Institute of Standards and Technology (NIST) database (https://webbook.nist.gov/chemistry/fluid/) and mutual solubility of CO2 and water based on the published laboratory experiments. We used the CMG STARS simulator as main solver, which has excellent performance in calculating heat exchange between fluids and rocks, and often is used to simulate thermal recovery processes in oilfields. To validate our results of viscosity and solubility inputs, we compare our model results with simulation results from compositional simulators CMG GEM and TOUGH2. These compositional simulators use their inbuilt libraries for fluid properties and their own interpolation algorithms (empirical relationships) for changing viscosity and solubility in defined P-T ranges. We then check the CO2 saturation and pressure results for different model scenarios in both CMG STARS, CMG GEM, and TOUGH2 to validate our main modeling approach in CMG STARS.

The comparison study and results show that our modeling technique achieves equivalent saturation and pressure values in the same injection production scenarios compared to verification simulators (CMG GEM and TOUGH2), where it outperforms by fully coupling the solubility and enthalpy. This modeling approach gives us the flexibility to prescribe fluid parameters that change at different pressure, temperature and brine concentrations. The model results reveal how the dense mixture of dissolved CO2 and formation brine moves in the reservoir and thus affects the reservoir's heat recovery scheme in long term.

Participation:

In-Person

References:

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Poster / 1065

Relationship between groundwater microtemperature and electrical potential of the vegetation

Authors: Maria Pinheiro[1]; Günter Buntebarth[2]; Martin Sauter[3]

[1] *University of Goettingen*

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The hydrological cycle is highly affected by changes in vegetation cover. One of the most important forces in this cycle is transpiration. This process returns approximately 50% of precipitated water back to the atmosphere, and accounts for more than 60% of the evapotranspiration rate. Vegetation is thus exposed to and governed by different meteorological variables, as well as by the availability of water in the soil and subsoil [1-9]. It's known that the variation in temperature of the groundwater at depths of up to 30 meters is subjected to daily and seasonal interference with the changing surface temperature. Beyond this depth thermal conductivity is not applied to detect signals of the surface temperature variation [10, 11]. However, groundwater microtemperature is clearly affected by vegetation activity [12-16].
The periodic variation in plant electrical potential has been evidenced in other studies [1, 17-19]. Some studies have shown that despite the periodic daily variation in electric potential in plants [1, 17, 20, 21], there is no direct link to xylem flow [17, 19, 22].
Atmospheric electricity has long been studied [23-25] and exhibits diurnal and seasonal variation [26]. While land and ocean tides are gravitationally controlled, atmospheric tides are mainly thermally controlled by solar radiation [27, 28].
The variation in groundwater microtemperature in summer was compared with meteorological parameters and with the electrical potential at plants. With increasing surface temperature, there is a decrease in relative humidity and an increase in the electrical potential of a tree, measured as the difference between the northern and the southern face of the stem (N –S), in order to eliminate the impact of the atmospheric electricity. This increase also coincides with an amplitude of approximately 2 mK in the groundwater temperature change and agrees with a vertical flow component of less than 10 cm. Possibly changes in the macro weather situation events were observed in the southern electric potential and groundwater temperature records. Atmospheric tides were detectable in the measurements of both, the north and south electric potentials.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS06-B / 1066

Use of surfactants to enhance the CO2 storage capacity in the geologic carbon storage

Author: Lee Joo Yong[1]

Co-authors: Ryou Jae Eun [2]; Min-Kyung Jeon [1]; Jongwon Jung [2]; Tae-Hyuk Kwon [3]; Park Yongchan [4]

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[2] *Chungbuk National University*

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Geologic carbon storage is the most readily available technique that can store the carbon in a relatively larger volume. The higher injectivity and the larger storage capacity are required for the efficient and economical geological carbon storage. The storage capacity of reservoirs highly depends on the multiphase flow properties of the reservoirs, especially the residual saturation of CO2 . The CO2-compatible surfactants can enhance the storage capacity by increasing the residual saturation of CO2, due to the reduced interfacial tension between brine and CO2 . A few groups of CO2-compatible surfactants have been tested for their performance in controlling interfacial tension in various pressure and temperature conditions. The interfacial tension and contact angle on commercially available substrate, such as quartz mineral and sandstones, were experimentally measured. The pressure and temperature ranges 25~40℃ and 4~10MPa, respectively. Non-ionic surfactants perform better than ionic surfactants in the brine-CO2 system, whereas the performances were similar to each other in the brine-air system. The contact angel alteration become more prominent in higher pressures. Lower interfacial tension and higher contact angle, induced from surfactants, will lower capillary pressure, and thus increase the residual saturation of CO2. The lower capillary pressure also enhance the sweep efficiency during the geologic carbon storage operation. Further study with various and systematic measurement conditions are required for the operation design in field scale.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

MS09 / 1067

Residual bubbles'local equilibrium after coarsening

Authors: Yuehongjiang Yu[None]; Chuanxi Wang[1]; Yashar Mehmani[2]; Ke Xu[1]

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Residual bubbles in porous media, initially emerging at non-equilibrium state by direct injection, phase changes or imbibition, spontaneously coarsen towards a thermodynamic equilibrium state. During coarsening process, bubbles'morphology and pore occupancy change that affects hydraulic conductivity, mass & heat transfer coefficients, and chemical reaction kinetics. The kinetics from initial distribution to equilibrium is critical in determining physically-correct models for predicting CO2 subsurface sequestration and gas condensate production.

Based on our earlier theoretical approaches on bubbles'coarsening [Xu et al., PRL, 2017; Xu&Mehmani et al., GRL, 2019] and on bubbles'stability analysis [Wang et al., PNAS, 2021], we apply recently-developed pore-network modeling (PNM) tool [Mehmani & Xu, JCP, 2022; Mehmani & Xu, AWR, 2022] to investigate the kinetics of bubble coarsening in porous media, and reveal the final state in both homogeneous and heterogenous media. The time scale of coarsening is also theoretically derived and numerically validated [Yu & Wang, et al., GRL, 2023].

We first study the local equilibrium state of a two-bubble system in two connected pores. Without external field, there are three different equilibrium states when increasing the initial bubble volume: (a)the smaller one is eaten by the larger one, (b)both bubbles survive but of different sizes, and (c)both bubbles survive and of the same size. When there is an external field, only (a) and (b) are found with the growth of initial bubble volume. Analytical solutions matches the simulation well.

We then simulate the bubble coarsening in a 200×200 homogeneous pore-network model. The results show that some bubbles survive and are all finally of the same volume while others disappear. Bubble coarsening kinetics in porous media deviates from Lifshitz-Slyozov-Wagner theory, showing a much slower radius –time scaling. We attribute this new scaling to that porous structure quantizes the space and decouple the mass transfer coefficient from the bubble size. We accordingly develop a new theory for bubble coarsening in porous media, that matches the theory well.

Finally, we investigate bubble coarsening in heterogeneous systems. Although slightly affected by initial condition, we note that survival bubbles at equilibrium statistically fill from the largest pore to smaller pores. We plot capillary pressure –saturation curve and pore-occupancy –saturation curve at equilibrium, that can well match our theory considering pore-size distribution. The time scale

for reaching equilibrium can also be estimated by the homogenous media theory, with necessary modification of perfector.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 1068

Transport in heterogeneously reactive media

Author: Dario Maggiolo[1]

Co-authors: Oskar Modin [1]; Angela Sasic Kalagasidis [1]

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Plume deformation and mixing determines the effective reaction in porous media
chracterised by internal heterogeneous reaction. Via pore-scale simulations, we show the dynamic of a passive scalar injected in a packed bed consisting of a mixture of chemically inert and reactive spherical particles (adorbers), to mimic, e.g., the contaminat uptake by a fraction of grains in the soil matrix 1.
The scalar plume deformation is a consequence of the different mechanisms of transport characterising the transport of molecules in the proximal and remote pores relative to the adsorbers, diffusion and advection, respectively. The scaling laws governing stretching and broadening of isoscalars are quantified and discussed in relation to medium characteristics, such as the mean adsorbers' interparticle distance.
We show that a transition from diffusion- to advection- dominated macroscopic adsorption is determined by the amount of adsorbers within the medium, with diffusion and advection dominating at high and low fractions, respectively.
At high fractions the temporal evolution of the macroscopic adsorption scale as $\propto \sqrt{t}$. while at law fractions it follows $\propto t$. The transition shows that more rapid adsorption is taking places in areas of soils where the fraction of adsorbers is lower, leading also to a faster saturation of contaminant uptake capacity.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

1069

The potential of sandstones from the Rio Bonito Formation, Paraná Basin, for implementing Carbon Capture and Storage in south-eastern Brazil.

Authors: Isabella Miranda[1]; Lucy Sant'Anna[2]; Colombo Tassinari[1]

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[2] *University of São paulo*

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The intense use of fossil fuels worldwide has increased the release of greenhouse gases (GHG) into the atmosphere, with carbon dioxide (CO2) being the main one. In this context, Carbon Capture and Storage (CCS) technology has been promoted over the last few years as a good long-term alternative to help countries reduce the emission rate of greenhouse gases, especially carbon dioxide (CO2). Despite having few projects, Brazil has advanced in CCS implementation studies, some offshore and others related to BECCS onshore. Implementing BECCS systems in the country may be very useful in reaching negative CO2 emissions, especially in the South-Southeast region, which concentrates the most significant number of bioenergy plants. In his favor, Brazil has an extensive area of continental proportions, encompassing several sedimentary basins prone to the application of CCS, such as the Paraná Basin. The Paraná Basin nestles sandy and clayey sedimentary units exhibiting significant lithological heterogeneity, such as those of the Rio Bonito Formation (Permian). The Rio Bonito Formation is approximately 350 meters thick and comprises sandstones, conglomerates, siltstones, coal, and carbonaceous shales, deposited in coastal to shallow marine environments. The Rio Bonito sandstones present great regional diversity in the Paraná Basin, resulting in different types of mineralogy and portions with higher porosity and others with lower porosity, as well as varied permeability. This Formation is the main oil play in the intracratonic Basin of Paraná, with characteristics of a suitable reservoir, even on a non-commercial scale. This work aims to characterize the sandstone layers of the Rio Bonito Formation to confirm if it is suitable for CCS reservoirs, based on mineralogy, porosity and permeability for implementing CCS in southeastern Brazil. Preliminary data suggest a positive potential of some sandstone portions for geological CO2 storage. This research is supported by the RCGI –Research Center for Greenhouse Gas Innovation, hosted by the University of São Paulo (USP) and sponsored by FAPESP –São Paulo Research Foundation (2014/50279-4 and 2020/15230-5) and Shell Brazil.

Participation:

Online

References:

Milani et al 2007; Schneider et al 1974

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Energy Transition Focused Abstracts:

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Poster / 1070

PTFE-based pore-filled ion exchange membranes for electrodialysis and energy conversion processes

Author: Jeong-Hoon Kim[1]

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Ion-exchange membranes(IEMs) have been widely used for desalinated and energy conversion processes. Since the IEMs determine the efficiency of the above process, it is necessary to develop them with impoved separation performance and durability. Novel composite-type anion- or cation-exchange membranes were prepared as follows; first, pore-filling of monomer mixtures (styrene/divinylbenzene (DVB), vinylbenzylchloride(VBC/DVB)) and an initiator was done in commercial polytetrafluoroethylene(PTFE) porous films, respectively. Thermal polymerization was followed in high temperature oven for the formation of precursor membranes. Post-sulfonation was done with chlorosulfonic acid in methylene chloride to give -SO3H for the preparation of cation exchange membranes. Post-amination was performed in trimethylamine (TMA) in acetone to give -N+(CH3)3- for the preparation of anion exchange membranes. SEM analysis confirmed these membranes were successfully prepared.
The electrochemical properties of the resulting membranes - ion exchange capacity, electric resistance and water content - were studied in terms of the ratio of dope compositions of monomers (Styrene/DVB, VBC/DVB).The composite membranes showed excellent electrochemical properties –electric resistance, water content and IEC value - depending on the monomer dope compositions (Styrene/DVB ratio and VBC/DVB ratio). These membranes showed lower electric resistances, lower water contents and higher IECs than commercial membranes thanks to thin PTFE supports. These results showed our composite membranes could be applied to the desalinatings electro-dialysis and energy conversion process.

Participation:

In-Person

References:

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2) Vijayakumar, V., Son, T. Y. & Nam, S. Y. Recent advances in composite polymer electrolyte membranes for fuel cell. Appl. Chem. Eng. 30, 1–10 (2019).
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Energy Transition Focused Abstracts:

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Poster / 1071

Waste Rock and Bentonite Mixtures for Gas Management within Low Heat Generating Waste Geological Disposal Facilities

Author: Elise Mouat[1]

Co-authors: Ian Molnar [1]; McDermott Christopher [1]; Bryne Ngwenya [1]; George Towler [2]; Clare Bird [3]

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[2] *Quintessa*

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The geological disposal facility (GDF) is the most common planned method for the disposal of radioactive waste. GDFs utilise a multi-barrier concept designed to prevent the release of radionuclides into the surrounding environment, collectively known as the engineered barrier system (EBS). The EBS is a key component for GDF safety as it slows the inflow of water to limit corrosion, protects the structural integrity of the container, and prevents radionuclides from being released into the environment.

The EBS also manages gases that are produced in the GDF during container corrosion and waste degradation, providing pore-space and passively controlling gas release to limit pressures and reduce the risk of gaseous radionuclide release. This project explores use of bentonite clay and waste rocks (WR) from quarries, excavated GDF rocks and re-use of other materials for the EBS. Their use as an EBS material would lower the environmental footprint and prevent these materials from filling landfills. We are assessing whether WR/bentonite mixtures meet criteria for EBS usage, including mechanical strength, fluid/gas permeability, microbial activity for gas consumption and the long term performance of these re-used materials. This is being conducted through a series of laboratory based and modelling techniques.

The use of bentonite in the EBS is internationally supported by several waste management organisations due to its high adsorption capacity, swelling properties and its low hydraulic conductivity. The addition of WR aggregate provides increased mechanical strength, improves gas permeability and increases the potential to host communities of gas-consuming microbes. This poster showcases the results from initial mechanical tests.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 1073

PE-based pore-filled ion exchange membranes for electrodialysis and energy conversion processes

Authors: Jeong-Hoon Kim[1]; Bo-ryung Park[2]

[1] *Korea Research Institute of Chemical Technololgy*

[2] *Korea Research Institute of Chemical Technology*

Corresponding Authors: brpark@krict.re.kr, jhoonkim@krict.re.kr

Ion-exchange membranes(IEMs) have been widely used for desalinating electrodialysis and energy conversion processes. Since the IEMs determine the efficiency of the above process, it is necessary to develop them with improved separation performance and durability. Novel composite-type anion- or cation- exchange membranes were prepared as follows; first, pore-filling of monomer mixtures (styrene/ divinylbenzene (DVB), vinylbenzylchloride(VBC/DVB)) and an initiator was done in commercial thin polyethylene(PE) porous films, respectively. Thermal polymerization was followed in high temperature oven for the formation of precursor membranes. Post-sulfonation was done with chlorosulfonic acid in methylene chloride to give -SO3H for the preparation of cation exchange membranes. Post-amination was performed in trimethylamine (TMA) in acetone to give -N+(CH3)3- for the preparation of anion exchange membranes. SEM analysis confirmed these membranes were successfully prepared.
The electrochemical properties of the resulting membranes - ion exchange capacity, electric resistance and water content - were studied in terms of the ratio of dope compositions of monomers (Styrene/DVB, VBC/DVB).The composite membranes showed excellent electrochemical properties –electric resistance, water content and IEC value - depending on the monomer dope compositions (Styrene/DVB ratio and VBC/DVB ratio). These membranes showed lower electric resistances, lower water contents and higher IECs than commercial membranes thanks to thin porous PE supports. These results showed our composite membranes could be applied to the desalinating electro-dialysis and energy conversion process.

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Energy Transition Focused Abstracts:

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Poster / 1074

Swelling of oak wood in water-ethanol mixtures : impact of the liquid composition on the material deformation.

Authors: Cédric Dussaut[1]; Julien Colin[2]; Joel Casalinho[1]; François Litoux-Desrues[3]; Rémi Teissier du Cros[3]; Charlotte Abadie[None]; Patrick Perré[1]

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Aging is a key milestone of spirits production during which mass exchanges occur between brandies and the external environment. The barrel is a complex porous media made of oak wood and acting as a container 1. During aging, the liquid present in a barrel partially impregnates the wood and migrates as liquid state. In the outer, non-impregnated part of the stave, vapour concentration gradients trigger diffusion. These mechanisms are responsible for a volume loss from 1% to 3% per year, depending mainly on environmental conditions [2]. In addition, wood is not an inert interface since the presence of water and ethanol modifies its physical properties.
The hygroscopic nature of wood is responsible for adsorption as bound phase when in contact with aqueous solutions or liquid ethanol. Such adsorption causes swelling of the wood due to its sub parietal macromolecular structure. In the case of barrels, the mechanical assembly of the staves hinders the free swelling of the wood and thus creates mechanical constraints that improve the sealing between staves. However, the coupled effects of water, ethanol and time on the cell wall are not fully understood. Because of the diversity of alcohol content of the brandies, it appears relevant to study the effect of the liquid composition on the wood swelling. Previous studies highlighted dimensional changes in pure ethanol to be lower than in pure water [3][4]. This work focuses on oak wood dynamics and equilibria when soaked in pure water, pure ethanol or binary mixtures. A custom device has been developed to determine the evolution of swelling in both transversal directions as a function of the liquid composition, through image processing. Eight ethanol concentration values have been tested from 0% to 100% (vol/vol). As shown in the attached figure (a), a synergic effect is evidenced for a wide range of concentration from 20% to 80% of ethanol (vol/vol). This is in accordance with previous studies that have reported a higher swelling than with pure solvents [3][5]. This suggests a collaborative action of sorption sites when both solvents are in sufficient quantity. To complete these experiments, we studied sequential scenarii namely pure water followed by pure ethanol and vice versa (b). Results show that wood slightly shrinks when put in ethanol after having swelled in water. Thus, it seems that only a part of the previously bound water remains adsorbed onto wood while another part is desorbed due to its affinity with ethanol. On the contrary, when the chronology of pure liquids is inverted, the previously mentioned synergic effect is observed leading to the same swelling values as for mixtures between 20% and 80% of ethanol (vol/vol). Such results emphasize the influence of the history between wood and liquids.
To complete the study, a Dynamic Vapour Sorption device will be used to obtain sorption isotherms of oak wood for both water and ethanol in gas phase. This equipment allows also to study the reversibility of interactions between wood and vapours.

Participation:

In-Person

References:

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Energy Transition Focused Abstracts:

Poster / 1075

Effect of fluids on micro-crack evolution in organic-rich shale by molecular dynamics simulations and nanomechanical experiments: A microscopic perspective from the fluid effect on fracturing

Author: Tianhao Wu[1]

Co-authors: Junliang Zhao [2]; Abbas Firoozabadi [3]; Dongxiao Zhang [1]

[1] *Eastern Institute for Advanced Study (EIAS)*

[2] *Southern University of Science and Technology*

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Hydraulic fracturing is a widely used technique in shale oil and gas development. As a promising method, CO2 fracturing has been suggested because of various advantages, including lower formation sensitivity, lower fracturing pressure, and higher fracture intensity. However, the mechanisms are not well-understood. One of the potential reasons is the strong interaction between the fluids and rock. In this study, the process of micro-crack evolution is investigated by molecular dynamics simulations and nanomechanical experiments. The effect of CO2 and H2O on the mechanical properties of typical components in organic-rich shale is analyzed. The strength and fracture toughness of solids in fluids are computed through molecular dynamics simulations. The results indicate that, due to the physical fluid-solid interactions, the mechanical properties of minerals and kerogen may change after exposure to fluids, which is different from geochemical processes. Based on the simulations and experiments, the changes in elastic modulus can lead to complex stress conditions due to swelling and shrinkage, and the presence of oil and gas can further complicate the behavior. The effect highly relies on the interfacial properties between fluids and shale. In the CO2-philic components (e.g., kerogen), the strength and fracture toughness may reduce by CO2 significantly. In hydrophilic constituents (e.g., clays), H2O has a more pronounced effect on mechanical properties than CO2. These findings suggest that CO2 can decrease the strength and fracture toughness of organic-rich shales, and micro-crack may propagate through CO2-philic components. This study provides a microscopic perspective on fracturing in shale, which may facilitate the improvement of the CO2 fracturing technique.

Participation:

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References:

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Poster / 1076

DeepAngle: Deep-learning-based estimation of the contact angle distribution in tomography images of porous media

Authors: Arash Rabbani[1]; Masoud Babaei[2]; Peyman Mostaghimi[None]; Ryan Armstrong[None]; Vahid Niasar[2]; Chenhao Sun[3]

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DeepAngle uses machine learning to determine contact angles between different phases in the tomography images of porous materials. The measurement of these angles in 3D can be inaccurate and time-consuming due to the discretized space of image voxels. A computationally intensive solution involves fitting and vectorizing all surfaces using an adaptable grid to measure angles between the desired vectorized planes. However, the present study offers an alternative low-cost technique that utilizes deep learning to estimate interfacial angles directly from images. DeepAngle was tested on synthetic and realistic images and was found to improve the r-squared of predicted angles by 5 to 16%, while reducing computational costs by 20 times. This rapid method is particularly useful for processing large tomography data and time-resolved images that are computationally intensive. The developed code and the dataset are available in a public repository on GitHub at [https://www.github.com/ArashRabbani/DeepAngle].

Note: An extended version of this poster has been accepted for publication by in Journal of Geoenergy Science and Engineering.

Participation:

In-Person

References:

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Poster / 1077

The Nature of Multiphase Flow in Microfluidic Devices

Authors: William Rossen[1]; Simon Cox[2]; Afshin Davarpanah[2]; Ewald Obbens[3]

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Microfluidic devices offer unique opportunities to directly observe multiphase flow in porous media. However, they face difficulties in representing steady multiphase flow without fluctuating occupancy of locations in the network. The ability of two phases to form steady, intertwined flow pathways is a key property of 3D pore networks (Sahimi, 1994; King and Masihi, 2019). This is not possible in a two-dimensional network (Fisher, 1961) unless the flow paths of the two phases can cross at some locations in the network. Crossings are possible in a microfluidic network if wetting phase can form a bridge across the top and bottom of a gap between grains at a pore throat while nonwetting phase flows through the throat, as illustrated below.

We examine the conditions under which this is possible using the Surface Evolver software (Brakke, 1992) to determine fluid interface shapes in several different throat geometries (Cox et al., 2023). For relatively long straight or curved throats, the most common geometry in microfluidic networks used for modeling flow in geological formations, the capillary pressure for bridging is the same as that for snap-off. This means steady two-phase flow is not possible in these networks without fluctuating occupancy of the pore space. In other words, flow is forced into a regime where phases displace each other in the network, even at the very lowest capillary number.

Concave throats, as between cylindrical barriers, can support bridges over a substantial range of capillary pressure. The range of capillary pressures at which bridging is stable increases as throats become more strongly concave (i.e., pillar radius decreases) and for narrower throats. Steady two-phase flow would be possible in networks of pores with throats of this geometry.

For networks of this geometry, we estimate the range of fractional flows of wetting and nonwetting phase that could be sustained. In addition to bridging, the geometry of the wetting-phase flow paths are complex. To get past pore bodies occupied with nonwetting phase, wetting phase is restricted to the corners at the top and bottom of the pillars, as illustrated below. We input flow geometries determined by the Surface Evolver into the COMSOL numerical flow solver to esimate relative permeabilities of both phases for a given network realization. We choose assumptions that favor the flow of the wetting phase: for instance, penetration of the nonwetting phase just to the point where it connects across the network. The results show that the relative permeability of the wetting phase is roughly 1/10 of that of the nonwetting phase. If viscosities of the two phases were roughly equal, that the maximum fractional flow of wetting phase would be 0.1. For gas-water studies, where the viscosity ratio can be 50:1, the maximum fractional flow of water would be 0.2%. Imposing a fractional flow above this would guarantee fluctuating pore occupancy in the network.

Participation:

In-Person

References:

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MS11 / 1078

Hydrate film formation in subsea carbon storage

Author: Wen Song[1]

Co-authors: David Fukuyama [2]; Hugh Daigle [1]

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Growth mechanisms of CO2 hydrates in pores dictate the capacity, injection rates, and long-term security of sequestered carbon. We reveal a previously unrecognized reactive transport mechanism dictating hydrate growth in pores: capillarity. Hydrate crystals, having superhydrophilic surfaces (θ~0°), form a secondary microporous medium (~ 100 nm pores) within individual lithologic pores (~ 10 to 100 μm pores) that promotes hydrate growth in a positive feedback cycle wherein water is imbibed spontaneously through the hydrate that forms at the water-CO2 interface. This self-reinforcing process drives hydrate film growth along the pore wall, and acts as a supply mechanism of water for hydrate formation in the gas-filled pores. The importance of capillarity on hydrate growth is validated experimentally and numerically through fluorescent imaging and by tracking the water phase movement during hydrate formation. Hydrate stability against temperature perturbations is provided by the endothermic nature of hydrate dissociation that would otherwise cause catastrophic release of CO2 from hydrate.

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1080

Characterization of water flow behavior during spontaneous imbibition in coal: From the perspective of fractal theory and NMR tests

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The spontaneous imbibition (SI) of water plays a crucial role in determining the wetting effect of water injection in coal seams. It is important to explore the flow behavior of water in coal during the SI. Contact angle measurement, SI experiment, and low-field nuclear magnetic resonance (LF-NMR) tests have been conducted to measure the properties of coal plugs from five different regions of China. The mass change of the coal by SI is related to the square root of time divided into three-stage linear functions in which the slope represents the imbibition rate of coal. The imbibition rate decreases with the increased SI time. The contact angle of bituminous coal is smaller than that of anthracite and is negatively proportional to the SI rate and capacity index C. Water is primarily stored in the adsorption and seepage pores, and little in microfractures. It shows that the fractal dimensions of the partial free pore (Db) and total pores (D) decline in a form of power law, while the fractal dimension of the free pore (Dz) declines irregularly. D-10 and D10 are strongly linear with the T2 spectrum area of adsorption pores, seepage pores, and microfractures, respectively. It indicates that e the low-probability measurement area represents the adsorption pores, and high-the probability measurement area represents seepage pores and microfractures. Adsorption pores play an important role during SI. The difference between the amplitude change of adsorption pore and that of seepage pores/microfractures is the key factor affecting multifractal parameters of T2 spectra. The linear relationship between H and Db reveals that water preferentially enters a pore with lower roughness and better connectivity during SI. The process of SI has been divided into three stages in terms of SI rate. The transport process of water within the coal at different stages has been discussed as well. The results of this work are of great significance for optimizing the coal seam water injection and reducing the risk of underground coal mine disasters.

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In-Person

References:

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Energy Transition Focused Abstracts:

1081

Poro-Elasto-Plastic Modelling of Hydraulic Fracturing in Natural Fractured Deep Reservoirs

Authors: Wenzhong Li[1]; Wenzheng Liu[1]; Chao Li[1]; Yu Wang[1]; Jianting Huang[1]; Yuanpeng Jiang[1]

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In this paper, a hydro-mechanical model is established to simulate the multiple hydraulic fractures propagation in naturally fractured deep reservoirs. The Drucker-Prager plasticity model, Darcy' s law, cubic law and cohesive zone model are employed to describe the plastic deformation, matrix flow, fracture flow and evolution of hydraulic fracture, respectively. The cohesive finite element method and return-mapping method are used to simulate the deformation of inelastic rock. The fluid flow in hydraulic fractures and matrix are modeled by the discrete fracture model (DFM) and finite volume method (FVM). In addition, a hybrid iterative algorithm is proposed to solve the strong nonlinear systems by a combination of the fixed-stress iteration, Picard iteration and Newton-Raphson iterative method. Then, the accuracy and ability of the proposed model are verified against analytical solutions of several classical reference cases. Finally, some numerical cases are conducted to investigate the influences of rock plasticity on the simultaneous propagation of multi-fractures and study the optimization of multi-fracturing of horizontal wells in deep reservoirs. Results show that plastic deformation greatly reduces the effectiveness of staged volume fracturing in horizontal wells. By appropriately optimizing the cluster spacing, not only the optimal reservoir reconstruction can be performed, but also the adverse effect of rock plasticity on fracturing treatment can be weakened by using the stress interference effect.

Participation:

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Poster / **1082**

Simulation of CO2 Injection and Development of Proxy Models for Svelvik CO2 Field Lab

Authors: Wilson Wiranda[None]; Ashkan Jahanbani Ghahfarokhi[None]; Cathrine Ringstad[None]; Alv-Arne Grimstad[None]

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Svelvik CO2 Field Lab is a small-scale field laboratory located about 50 km southwest of Oslo in Norway. The test site occupies an inactive part of a sand and gravel quarry, located in a glaciofluvial –

glaciomarine environment. It consists of an injection well surrounded by four monitoring wells covering an area of approximately 300m x 150m. The injection well facilitates water and CO2 injection at a depth of 64-65m. From September to November 2019, through the Pre-ACT project (Pressure control and conformance management for safe and efficient CO2 storage –Accelerating CCS Technologies), an injection campaign was performed. The data sets gathered from this campaign are geophysical monitoring of the CO2 plume (seismic and ERT), water and CO2 injection rates, and pressure at the depth of injection for the injection well and the monitoring wells. By using this data, numerical simulations of CO2 injection at Svelvik CO2 Field Lab were performed. To capture the CO2 plume movement, a fine grid geological model was used in the simulation study which takes seven hours to complete the Pre-ACT injection.
In this study, an initiative is proposed using proxy models to reduce the simulation time and to be used for the next injection design. A prediction scenario of two cycles with one week injection and one week shut-in is recommended for the proxy model development. By using the history-matched model, 18 different injection cases with different CO2 injection rates were simulated by using a numerical reservoir simulator. The results from the numerical reservoir simulator were used to train the proxy models. The proxy models used in this study are response surface proxy and universal kriging proxy with the input of first and second cycle CO2 injection rate. Several outputs are predicted using the proxy models, such as injection bottomhole pressure, average field pressure, field dissolved CO2 in water, and field CO2 in the gas phase. The validity of the proxy models is evaluated by percent error and correlation coefficient (R2).
The results of the response surface and universal kriging proxies show promising results for the evaluation and validation cases. All predicted results have R2 greater than 0.99, which means that the proxy models are highly correlated to the simulation results. The universal kriging proxy shows a better performance than the response surface due to the limitation of the response surface in following the polynomial regression model, while the universal kriging has the potential to minimize the error through the Gaussian process.
Overall, this study presents a success story of proxy model implementation in CO2 injection to replicate key results from the numerical simulations. Moreover, the proxy model can reduce the time required to complete a numerical reservoir simulation, which is an advantage in performing experiment design for the next injection in Svelvik CO2 Field Laboratory.

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In-Person

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1083

Digital core on a chip

Author: Dmitrii Pereponov[1]

Co-authors: Alexander Avdonin [2]; Michael Tarkhov [3]; Vitaly Kazaku [4]; Vladislav Krutko [2]; Alexey Cheremisin [1]; Evgeny Shilov [1]

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The development of hard-to-recover oil and gas reserves every year requires ever-more-innovative approaches for the efficient production of hydrocarbons. The petroleum industry has recently turned to the use of microfluidic technology for the laboratory investigation of the fluids'interaction under reservoir thermobaric conditions. The idea of this study lies in a development of a methodology for creating a porous microfluidic chip structure with properties that closely resemble those of the real deposit. To achieve this, we constructed a high-quality digital model of the pore space using advanced technologies such as high-contrast CT scanning, FIB-SEM technology, and the Navier-Stokes-Brinkman hydrodynamic solver. By adding all the 3D layers along a given axis, we obtained a 2D image that was subsequently segmented by a local median filter, expansion, and erosion operations. This image formed the basis of the porous structure of the silicon-glass microfluidic chip, which allowed us to experiment under high pressures and temperatures. The pore size distribution of the model was found to be in complete agreement with the distribution of the core, which confirmed the accuracy of the executed structure. Several experiments were conducted on the microfluidic chip, which helped determine the permeability value of its porous medium. The experimentally obtained value was validated on Geodict and in-house software in 2D and 3D projections. Furthermore, we performed a microfluidic test for pure n-decane and water, followed by the calculation of the displacement coefficient. Additionally, for the microfluidic chip, a detailed SEM scan was done with a large magnification, and subsequent watershed segmentation that proved similarity of the model with a real manufactured microchip. All in all, the symbiosis of two advanced technologies, microfluidics and digital core modelling, has facilitated in even greater benefits for the petroleum industry from laboratory research. This approach has allowed to significantly speed up laboratory tests, reduce their cost, and enable the validation of newly created software for numerical simulation.

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Online

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Poster / 1084

CAN SINGLE POROSITY MODELS ADEQUATELY REPRESENT HEAT FLOW IN FRACTURED POROUS MEDIA?

Author: David Egya[1]

Co-authors: Daniel Arnold [1]; Sebastian Geiger [2]

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Understanding of heat transfer processes in subsurface fractured rocks is critical for the development of geothermal resources. One of the challenging tasks is to build models that can adequately represent the complexity of the formation geometry and subsurface processes without the extensive computation cost. Single porosity models with effective parameters are commonly used for this purpose. However, these models are often too simplistic and inadequate to represent complex fractured rocks. The aim of this study is to evaluate when a single porosity model can adequately represent heat flow in fractured rocks. Our study uses numerical modelling to simulate heat flow and upscale hydraulic and thermal properties. We then use thermal breakthrough curves generated from the simulation results to evaluate the performance of the upscaling. Embedded discrete fracture model (EDFM) with explicit fracture and rock properties provides the base solution with which we evaluate the performance of the single porosity model. Our sensitivity analysis includes fracture density, connectivity, fracture lengths as well as the permeability contrast with the background matrix. The results indicate that single porosity models are mostly inadequate to reproduce the thermal breakthrough of fractured rocks except for cases where the permeability contrast between the fractures and the matrix is less than three order of magnitude. Overall, this study demonstrates when a single porosity model can be useful to represent heat flow in fractured rocks.

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In-Person

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1085

The Anisotropic Wooding Problem

Authors: Islam Shamima[1]; M Ferdows[2]; Rees Andrew[3]; P. Bassom Andrew [4]

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We consider the Wooding problem, which consists of a semi-infinite porous medium which is heated from below and in which the overlying cold ambient fluid is drawn uniformly downwards through the bounding surface. Our aim is to determine the effect of mechanical anisotropy of the medium on the onset of convection. To this end, a linear stability theory is developed and solved using standard numerical methods. The degree of anisotropy is measured by the permeability ratio, ξ, which is the ratio of the horizontal and vertical permeabilities. We present the variation of the critical Darcy-Rayleigh number and wave number with ξ. Using an asymptotic analysis it is also

found that the critical wave number tends towards being proportional to ξ^{-1/4} as ξ increases without bound.

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Poster / 1086

Characterisation of porous biochar using X-ray micro-CT and FTIR techniques

Authors: Pavel Kazakovtsev[1]; Tannaz Pak[1]; Kamal Elyasi Gomari[None]; Guoting Li[2]

[1] *Teesside University*

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Biochar is a carbonaceous porous material with wide range of applications. Biochar is produced via pyrolysis of organic material such as agricultural or forestry waste. Some examples of possible applications are fertiliser production, carbon storage, and water/soil decontamination (Cao et al., 2009). Biochar can be produced from waste material, such as manure, sawdust, or wastewater sludge (Chen et al., 2021). This makes biochar especially valuable, as it allows to recycle waste along with production of useful material. This also proves useful when we speak of net zero economy. Decomposing biomass emits carbon dioxide in the atmosphere while pyrolyzing it into the biochar allows to capture carbon in the solid form for centuries.

This work studied the possibilities to use brown algae as a feedstock for biochar production, as it can be grown year-round, at a rapid rate due to natural plant properties (Singh et al., 2021). With the ongoing climate change and resulting eutrophication, the total amount of brown algae in the sea has increased. This excess algae growth offers an excellent opportunity if it can be converted into some useful and valuable material (Zhao et al., 2022). An added benefit of using brown algae as a feedstock for biochar production is that algae do not compete with traditional terrestrial sources of biomass. Important factors to consider here are competition with food crops, land use, and fresh water use. For this study, two species of brown algae were selected - Laminaria Digitata and Pelagic Sargassum. The algae were pyrolyzed at temperatures of 300 ℃, 600 ℃, and 800 ℃. Samples pyrolyzed at 600 ℃ were additionally chemically activated with potassium hydroxide (KOH).

The X-ray micro-CT study was performed on the biochar samples to measure the porosity and, using pore-network modelling, to calculate the permeability of the samples. In addition to that, similar study was performed on commercial biochar (SoilFixer) to compare their properties. To better understand the chemical composition of the biochar, and if there are differences between the activated and non-activated biochar samples, a study with Fourier-Transform Infrared Spectroscopy (FTIR) was performed.

As a result of the X-ray micro-CT study, it was concluded that algal biochar is heterogeneous, with large mineral deposits in the structure. Additionally, it was shown that despite being of the same species, porosities measured for different (mm scale) samples were not necessarily similar. This

stands true for algal and wooden biochar. Distribution of porosity along the sample, however, was more homogeneous for wooden biochar.
The FTIR study showed that spectra produced for the biochar samples were similar, which may signify that there is a common compound in the algae, which influences the spectra, such as cellulose.

Participation:

In-Person

References:

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Zhao, M., Ma, X., Liao, X., Cheng, S., Liu, Q., Wang, H., Zheng, H., Li, X., Luo, X., Zhao, J., Li, F. and Xing, B., 2022. Characteristics of algae-derived biochars and their sorption and remediation performance for sulfamethoxazole in marine environment. Chemical Engineering Journal, 430, p.133092.

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1087

Splitting schemes for multiscale multicontinuum problems in fractured porous media

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This work considers the coupled system of equations that describe flow in fractured porous media. To approximate by space, we use a finite volume approximation with an embedded fracture model to simulate large thin fractures (hydraulic fractures) and a dual continuum (dual porosity dual permeability) approach for natural fractures. Such models are similar and can be described using the multicontinuum approach. The main goal of the work is to develop, analyze and investigate an efficient decoupling scheme that allows separating equations for each continuum. The approach is based on the semi-implicit approximation by the time where the coupling part between each continuum is taken from the previous time layer. We apply and analyze this approach for classical multicontinuum problems in fractured porous media on regular, sufficiently fine grids. We show that the presented scheme is stable, accurate, and computationally efficient. Presented decoupled schemes separate the continuum, and the resulting equation in a sequence requires a smaller number of iterations.
Next, we consider a multiscale approximation, where the same multicontinuum approach can be used to construct an accurate reduced-order model by space. We construct the multicontinuum upscaled models based on the nonlocal multicontinuum (NLMC) method, where multiscale basis functions are calculated in a local domain for each continuum. Numerical results show that the presented scheme for the NLMC method provides an accurate and efficient upscaled model on the coarse grid.

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Poster / 1088

Alquimia: A generic interface to biogeochemical codes

Authors: Sergi Molins[1]; Benjamin Andre[None]; Glenn Hammond[None]; Jeffrey Jonhson[None]; Benjamin Sulman[None]; Konstantin Lipnikov[None]; Marcus Day[None]; James Beisman[None]; Daniil Svyatskiy[None]; Carl Steefel [1]; John David Moulton[2]

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Multicomponent reactive transport codes couple biogeochemical models with solvers for flow and transport and other relevant processes. Many of these codes are the legacy of years of development and research, over which model complexity has increased incrementally. Often the complexity of implementing a comprehensive and flexible treatment of biogeochemistry is a significant obstacle to the development of new biogeochemical capabilities. As a result, this step is often circumvented by coupling flow and transport codes to existing biogeochemical codes. However, this is typically done as a one-off to a specific code. In this poster presentation, Alquimia, an open-source software library is introduced that provides a generic interface to existing biogeochemical capabilities. This software is intended to facilitate interoperable code development by exposing tried-and-true biogeochemical capabilities in existing software. To exemplify its use, the geochemical capabilities in the open-source reactive transport codes PFLOTRAN and CrunchFlow are made available via Alquimia's generic interface. This interface is then used to add geochemical capabilities to Amanzi and ParFlow. We show that because Alquimia allows for different geochemical codes to share flow and transport solver, and therefore the same spatial discretization, time stepping control, and coupling schemes, it may be a useful tool for benchmarking. We also present examples of how Alquimia has enabled incorporation of geochemical capabilities to codes for a range of applications.

Participation:

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Energy Transition Focused Abstracts:

1090

Early-time dynamics of negatively buoyant plumes in porous media

Authors: Sibasish Panda[1]; Chunendra K Sahu[2]

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The occurrence of negatively buoyant plumes in various real-world scenarios has rendered it a relevant topic in research. For example, solute transport and dispersion of contaminants in subsurface flows are defined by plumes. We perform a series of laboratory experiments to study negatively buoyant plumes in homogeneous porous media. The experiments are performed in a large transparent tank to minimize the boundary effect. We inject dyed salt water at the top surface of the medium, which is saturated with fresh water. To imitate a wide range of flow conditions, we study the effects of variation of reduced gravity, inflow flux, and permeability. During experiments, high-resolution images of the running plumes at regular intervals are captured using a DSLR camera. We use the dye attenuation technique for flow visualization, where calibration experiments are performed prior to starting the plume experiments to relate the injected dye concentration with the light intensity. The calibration curve obtained from these experiments is then used to obtain concentration maps of the plume in the flow domain. Subsequently, through image processing with in-house MATLAB code, we determine an optimal threshold to find the interface between the injected fluid imitating the contaminant and the ambient in the saturated media. Figure 1 shows the evolution of the plume for a sample experiment and also draws a parallel between the plume interface in captured images and concentration maps

Following the extraction of relevant data, we investigate the extent of longitudinal length and volume spread with time. Additionally, we classify the plume as - “Early plume” and “Transitioning plume” and define a “transition time” based on its flow regime. We propose a semi-empirical model correlating the length and volume spread of the plume with time and experimental parameters such as flux, reduced gravity and permeability, and transition time for both the flow regimes with the same set of parameters. Analysis of the proposed model with the obtained experimental data shows a good agreement. We find an equation correlating dimensionless length with dimensionless time of the form $\hat{L} = 23.79 q^{1.73} g'^{-1.75} k^{-2.07} \hat{t}$, where $\hat{L}$ is the dimensionless length, $p_0 = 23.79$ is the experimental constant, q is the flux, g' is the reduced gravity, k is the permeability and $\hat{t}$ is the dimensionless time. Similar correlations, to be discussed in the talk are also formulated, for volume spread and transition time. The talk will also briefly highlight research gaps in previous studies and conclude with discussion of prospects and applications of the study in subsurface flows.

Figure 1: Temporal evolution of a plume, along with its concentration maps.

Funding acknowledgment: SERB, DST, Government of India.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

Poster / 1091

Model for the simulation of reaction-mixing processes at boundary layers

Authors: Alisdair Soppitt[1]; Mohaddeseh Mousavi Nezhad[2]; Thomas Hudson[3]

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Reactive boundary conditions are employed to model an increasingly wide range of transport scenarios. While the capability of a variety of computational schemes for reliable description of such reaction-diffusion processes at the boundary of a given domain has been assessed in the literature, the effects of hydrodynamic processes on the rates of reactions taking place at the boundary are still largely unexplored.
We present a computational algorithm to model the turbulent mixing and transport of scalars through a channel in the presence of reactive boundary conditions, and obtain a pdf of their concentrations through time and space. A Lagrangian stochastic particle technique is used to model scalar transport. We consider a system with a partially adsorbing boundary condition modelled through the coarse-graining of small scale linear reactions. We observe a nonlinear dependence of the boundary reaction (i.e., sorption) rate on the turbulent frequency.

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Poster / 1092

Anisotropic stochastic Pore Network generation algorithm with application to shale gas flow

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With climate change mitigation actions in place, Carbon Capture and Storage (CCS) is by far the most industrially efficient technology to reach net-zero carbon emissions (HM Government, 2018), with current annual capture capacity exceeding 40 million tonnes of CO2 world-wide (BP, 2020). While supercritical CO2 is stored in conventional reservoirs or saline aquifers, overlying mudrock formations create a structural trap, preventing CO2 leakage. Opalinus Clay is a perfect candidate for CCS research, with a large amount of existing data (Bossart and Milnes, 2017) and experimental work performed, allowing for good understanding of pore space processes. Upscaling properties such as absolute and relative permeabilities and capillary pressures are necessary for reservoir-scale modelling of CCS processes and caprock leakage assessment, but are difficult to obtain experimentally.

Pore Network Modelling (PNM) is a method used for estimating representative rock flow properties, and is significantly more computationally efficient than most other methods. In this work we created an algorithm, which generates a representative pore space model with pore sizes ranging from sub-nanometre to over a micron, while carefully calibrating pore geometry to match observed porosity and pore size distributions. Novel technique for representation of the shale pore space anisotropic behaviour, which allows for adjustment of the degree of orientation of pore throats with respect to the bedding plane, based on Small-angle X-Ray Scattering observations. Real gas and adsorption effects were accounted for following the method used in (Song et al., 2018) and using experimental high-pressure sorption data respectively. Single phase gas permeability was simulated at various conditions and verified against unsteady state plug permeability measurements, performed on Opalinus Clay.

Participation:

In-Person

References:

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1093

A Layer Discrete Fracture-Matrix Simulation for Production Data Analysis in Well Intercepting Fractures in Multi- layer Tight Gas Reservoirs

Authors: Chengwei Zhang[None]; Shiqing Cheng[1]; jing Xu[2]; Xuesi Shen[3]; Chong Zhang[4]; Tingting JIANG[5]

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Multi-layer tight gas reservoirs have played a most important part in the development of tight gas reservoir. As we know, the separate layer hydraulic fracturing is very essential to multi-layer tight gas reservoirs. Therefore, the production performance analysis of tight-gas separately fractured well is important for us to study. However, until now, few researchers focused on layer discrete fracture-matrix(DFM) model. To supplement this disadvantage, this work proposes a layer DFM model to improve this situation. Considering that discrete fracture-matrix model is very useful for us to do our research on the well performance analysis about fractured well, this study uses a Layer DFM model based on the FVM-TPFA and Automatic-difference (AD) to do some research on the analysis of fractured well's production data analysis on multi-layer tight sandstone gas reservoirs. In this paper, a Layer Discrete fracture–matrix method is based on numerical simulation model (DFM-PDA). And it also provides an accurate code for the simulation of gas flow, including gas transport, and non-linear gas properties coupling in unconventional fractured gas reservoirs.
First, we present a new application of the FVM-TPFA formulation to model well performance about gas flow in hydraulically fractured multi-layer tight sandstone gas reservoirs containing hydraulic fractures by use of layer discrete fracture-matrix method. Then, the resulting system of equations is solved simultaneously for fracture, matrix and boundary conditions by use of finite volume method, two point flux approximation and automatic difference for pressure-dependent nonlinear terms such as density, viscosity and compressibility. Numerical examples and field cases are presented to test the validity and show the capabilities of the proposed approach. Compared with the conventional DFM model, the proposed model (layer DFM) is much more reasonable than it. And then proposed model provides a general framework that can be applied to a well intercepting multiple fractures and other multiple operating schedules, and it is used to analyze complex behaviors for gas wells. This layer DFM-PDA is verified through a commercial simulator. It can be applied in the performance analysis of well intercepting multiple fractures in Shenmu gas field. Not only in a way can this framework solve the problem in which nonlinear, pressure-dependent gas properties are captured without approximation, but it also can overcome the limitation of conventional DFM model.

Participation:

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Poster / 1094

Numerical Modeling of Two-Phase Flow in the Porous Pavement Drainage Structure

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A numerical model is developed to simulate the drainage process of porous pavements. The aim of this work is to gain a deeper understanding of the underlying processes and the relevant influencing parameters.
Porous pavements, such as porous asphalt (PA), are characterised by their high void content and are increasingly used in Germany and many other countries on highly congested roads outside urban areas due to their ability to reduce and absorb traffic noise. PA can achieve almost complete infiltration of all rainfall, with the water draining along the underlying dense layer. As a result, it increases road safety significantly (prevention of aquaplaning, splash and spray and glare by reflecting light), reduces and delays peak runoff during heavy rainfall events, and additionally traps pollutants to a certain extent.
The model is developed in the open-source simulation environment DuMuX and validated with measurement data and a simpler numerical model for the coupled drainage behaviour of porous asphalt available in the literature.
A parameter study with the model investigates the influence of road parameters (e.g. transverse/longitudinal slope, roadway width, as well as porosity and its decrease in the life cycle of the roadway due to clogging) on the drainage process. Additionally, reduction or delay of peak runoff with the help of PA compared to conventional wearing courses is analysed.

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References:

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Energy Transition Focused Abstracts:

1095

Experimental study on the wettability of tight conglomerate from Mahu Depression, Junggar Basin, Northwest China

Authors: Jianbang Wu[1]; Yang Shenglai[2]; Li Qiang[2]

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Wettability plays a crucial role in reservoir exploration and production by determining the microscopic distribution of fluids in rock channels. However, characterizing and understanding wettability in tight reservoirs remains a challenge due to the complexity of pores and minerals. In this study, Baikouquan and Wuerhe Formation core samples from the Mahu oil reservoir in China were used to conduct wettability evaluating and aging experiments through apparent contact angle and nuclear magnetic resonance (NMR) T2 spectroscopy. The cores were vacuumed and saturated with formation water, replaced with manganese water and simulated crude oil, and aged at high temperatures for 2-8 days. T2 spectra were utilized to monitor this process. Two contact angle tests were conducted on fresh and aged surfaces. The research revealed that the fresh rock surface of the tight sandy conglomerate samples are water-wet, but after aging, it becomes neutral to oil-wet due to crude oil peeling off the water film at high temperatures, allowing it to to approach the walls of the pore and enter the capillary depth. The physical and lithological properties of the core collectively influence wettability, with the presence of quartz enhancing hydrophilicity in the fresh state, and higher clay mineral content resulting in stronger hydrophilicity after aging. The physical property of the sample affects wettability, with tighter samples exhibiting higher hydrophilicity due to crude oil migration difficulty through micropores. A wetting index model was established using T2 geometric mean and T2 cutoff as a function of saturation, which correlated well with the wetting angle test results. The difference in the results of the two methods is related to the trapping capacity of the rock surface for the wetting phase.

Participation:

Online

References:

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Energy Transition Focused Abstracts:

Poster / 1096

Exploring the Impact of Ice Formation on Soil Temperature for Ground Source Heat Pumps

Authors: Ekaterina Lgotina[1]; Simon Mathias[1]; Marti Lloret-Cabot[1]

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Soil temperature is a key parameter defining the coefficient of performance (CoP) for shallow burial ground source heat pumps (GSHP). Whilst many studies incorporate the effects of temperature attenuation due to conduction and temperature reduction due to evaporation, few studies incorporate the effects of latent heat of fusion associated with ice formation/thawing. This latter effect will be more important in areas experiencing continental climates, where GSHP is considered to be particularly attractive.

Our project concerns developing an appropriate numerical modelling framework to explore the impact of ice formation/melting on GSHP-CoP. As a simple first step, we developed a heat conduction model accounting for moisture freezing and thawing combined with evaporation. The water is assumed immobile within a rigid solid porous matrix. Water within the soil matrix exists as either ice or liquid. Gains and losses of heat due to ice formation/thawing, respectively, occur throughout the model domain. Loss of heat due to evaporation occurs only at the soil surface, with water being instantaneously replaced such that the total mass of water in the system remains constant. The water (both ice and liquid) and soil are assumed to be in local thermal equilibrium. The resulting partial differential equation (PDE) uses specific internal energy as the primary dependent variable. Numerical solution is achieved using the method of lines.

An important factor that appears during the phase transition is the melting point temperature depression. Researchers mainly use a modified version of the Clapeyron equation known as the *generalised Clapeyron equation*, which estimates the equilibrium relationship between the temperature and pressure in freezing soils. Modifications to the original Clapeyron equation have been considered necessary because of potential misunderstandings about how matric potential (the capillary suction associated with soil pores) affects the melting temperature of ice.

To explore these ideas further, we studied the process of freezing of compressible water in a rigid tank of constant volume. The classical Clapeyron equation was coupled with the specific water volume functions to obtain two coupled ordinary differential equations (ODEs). These equations were then extended to consider freezing of water in a porous medium using constant rock properties and a uniaxial strain assumption. By solving the ODEs we were able to plot freezing point temperature as a function of liquid water volume fraction for different rock compressibilities.

Our preliminary simulations demonstrate important aspects concerning the effect of ice on soil temperature. The presence of ice leads to significant delays in changes in temperature around the melting point. Furthermore, heat conduction within the ice is faster due to its higher thermal diffusivity as compared to liquid water. There is also a significant difference between how the liquid water volume fraction depends on freezing temperature for the rigid tank model with and without uniaxial strain condition. It is expected that such effects will have a significant impact on GSHP-CoP. Future work will involve incorporating a more accurate representation of liquid and vapour movement within the soil as well as the effect of salt on the melting point depression.

Participation:

In-Person

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Energy Transition Focused Abstracts:

Poster / 1097

Characterization Of Capillary Driven Flow In Layered Porous Reservoirs

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Co-author: Jyoti Phirani [2]

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For gas storage in the geological reservoirs, it is important to understand fluid flow behaviour when capillary forces are dominant i.e. after the gas injection stops. In this work, we use numerical simulations to understand the capillary driven flow in layered porous reservoirs at Darcy scale. Using our model we want to predict if capillary breakthrough is possible in the cap rock based on the properties of the layers. We used MATLAB Reservoir Simulation Tool (MRST) for unidirectional capillary driven flow assuming horizontal displacement in co-current mode. The core dimensions of 5 m x 1 m x 1 m are used for two-layered reservoirs. We placed an additional grid cell of pore volume ten times to that of the core at one end of the setup which acts as a water tank. The boundary conditions in simulation are controlled using the wells. We positioned one injector well in the water tank and one production well at the other side of the core with pressures of both the wells being the same to allow for capillary driven flow. For a single layered, homogeneous system, we compared the obtained saturation profiles from the simulation with the analytical solution published in the literature. Comparisons are provided for three different wettability states for oil-water systems. For mixed wet case, the numerical solution shows a good match with the analytical solution. We validated our simulation model using several cases of the homogeneous reservoirs of different petrophysical properties, relative permeability, capillary pressure - saturation curves, and varying mobility ratios. Using our model for layered porous media, we observed that the fluids propagate with different velocity in each layer and wetting fluid (i.e., water for strong water-wet) reaches farther through the low permeability layer due to high capillary forces. The solution obtained can be used to study the influence of wettability, predicting saturation profiles and breakthrough characteristics. The simulation study undertaken can be used to understand the flow of wetting and non-wetting fluids in a geological layered reservoir, for example in CO2 sequestration when CO2 injection has stopped. Using this model we can estimate the required properties of the caprock for no leakage of CO2.

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