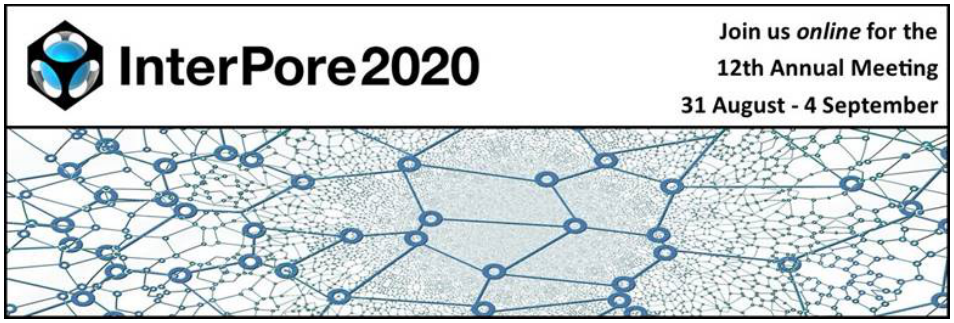
InterPore2020

Monday 31 August 2020 - Friday 4 September 2020



Book of Abstracts

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2

Various Mathematical Approaches to Mechanical Simulations in Wound Healing Processes

Authors: Fred Vermolen[1]; Qiyao Peng[1]

[1] *Delft University of Technology*

Corresponding Authors: f.j.vermolen@tudelft.nl, q.peng-1@tudelft.nl

Deep tissue injury often results in contraction of skin due to mechanical pulling forces exerted by skin cells in the dermal layer. If contractions are morbid, then they are referred to as contractures. Contractures cause disabilities to the patients, by, for instance, loss of mobility of a joint. By the use of modeling, we aim at understanding the mechanisms behind the formation of a contracture and at predicting which wound is likely to develop a contracture and which treatments can be employed to minimize the likelihood of a contracture. Since the cells are much smaller than the domain of computation, we used the immerse boundary approach based on a superposition of Dirac Delta functions to describe the forces exerted by individual skin cells. The use of this superposition of Delta functions results in a numerical solution that is not in H1. Hence, other alternative approaches are developed to avoid it.

In particular, to describe contractions during wound healing, the forces exerted by cells are actually applied on a continuous curve. Therefore, the region covered by the cell is modelled as a hole in the domain, then the surface forces at the cell are formulated by means of a force boundary condition. The last-mentioned approach shows consistency with the immersed boundary approach, which is proved both analytically and numerically. All the simulations and results will eventually contribute to modelling the contractions of the wound.

On the other hand, we are hunting for the approaches in a general perspective which entail smoothed Dirac Delta distributions. Additionally, we also analyzed a homogenization approach based on Green's fundamental functions. A Gaussian regularization is widely used as a replacement of Dirac Delta distribution. In this approach, the selection of the variance has a significant influence on the solution. For one dimension, it is relatively straightforward to demonstrate convergence of the Gaussian distribution approach to the solution using Dirac Delta distribution as the variance is decreasing.

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7

Geothermal Brine Reinjection from SaltPower Generation: A Microcalorimetry Study

Authors: Jacquelin Cobos Mora[1]; Erik Gydesen Søgaard[2]

[1] *Chemical Engineering and Biotechnology, Aalborg University*

[2] *Department of Biotechnology, Chemistry and Environmental Eng, Aalborg University*

Corresponding Authors: jec@bio.aau.dk, egs@bio.aau.dk

Geothermal water from Gassum sandstone aquifer has provided renewable energy in Denmark since the late 1970s . Normally the heat depleted brines are reinjected back into the same aquifer as a disposal solution. In recent years, it has been shown that hypersaline fluids can be used to produce energy by pressure retarded osmosis (PRO). The energy production from hypersaline fluids is called

SalPower electricity generation, which is based on the osmotic pressure difference between the draw (brine) and the feed (freshwater). By pressurizing the draw solution, a hydro turbine can convert the water flux across a semipermeable membrane into electricity \cite{Madsen2017}. Power densities above 5 W/{m^2} can be obtained if the PRO process is operated at pressure up to 70 bar. The idea of harvest more energy out of the heat depleted geothermal brines is attractive. The main issue with the overall process is the larger amounts of diluted brine that shall be handled. Reinjection can be considered as a feasible solution; nonetheless, the complex fluid-fluid and rock-fluid interactions that are taking place upon reinjection should be addressed properly in order to avoid technical and environmental issues. The present study aims to determine the implication of those dynamic interactions in a possible injectivity reduction (formation damage) due to diluted geothermal brine reinjection.

Isothermal titration calorimetry (ITC) can provide insights into complex fluid-fluid and rock-fluid interactions that can occur upon diluted geothermal brine reinjection. According to Cobos et al.\cite{Cobos2018}, ITC is a highly sensitive microcalorimetry technique that provides accurate adsorption enthalpy values which are used to elucidate the interfacial-phenomena at the rock-aqueous interface. In the ITC experiments, 100 mg of Berea sandstone powder ($<$ 100 μg) was placed in a reaction vessel and 200μL of Thisted geothermal brine (TB) was added to the particles. The titration ampule was lowered step by step into the calorimeter until it reached its final position. 10 injections of 9.948 μL of two times diluted brine (2D*TB) were titrated into the calorimetric cell after 1 hour of equilibrium time.

The result of the salinity difference between the injected fluid (2D*TB) and the formation brine is dynamic fluid−fluid and rock−fluid interactions. It was found that a water-water network perturbation occurred when 2D*TB was added to the sandstone−formation water system. On the other hand, an ion exchange process between the rock and the injected fluid also took place inside the porous media. A set of composition variation changes could stabilize the clay particles that are loosely attached to the pore surface. This is because 2D*TB has a lower ionic strength than TB. Consequently, polyvalent cations can be adsorbed onto mineral lattice while monovalent cations are being desorbed to keep the equilibrium in the solution. The direct implication of those dynamic interactions is a reduction in the possible formation damage as shown in \cite{Kia1987}. The authors acknowledge that special care should be taken when designing a reinjection scheme to avoid Fe(III) oxides precipitation inside the porous media.

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Pore-scale Investigation of Effects of Organic-matter Pores on Shale Properties Based on Multicomponent and Multiscale Digital Rocks

Authors: Yuqi Wu[1]; Pejman Tahmasebi[2]; Chengyan Lin[1]

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

[2] *University of Wyoming*

Corresponding Authors: lincy@upc.edu.cn, ptahmase@uwyo.edu, wuyuqi150348@163.com

Organic-matter (OM) pores play a significant role in the pore systems of shale formations. Numerous studies have analyzed the characteristics of OM pores. However, fewer studies reported the effects of OM pores and their chemical properties on shale properties. In this study, a comprehensive pore-scale investigation of the impacts of OM pores on various petrophysical properties based on multicomponent and multiscale shale models is presented. To this end, a novel technique for constructing three-dimensional (3D), multicomponent, and multiscale shale models is proposed. Multiple shale models with different fractions of OM pores are then generated using the proposed algorithm. Based on these shale models, the effects of OM pores on the geometric, topological, and transport properties and correlation functions of pore space are comprehensively evaluated within the physics-based and realistic models. The results show that the addition of OM pores in the pore systems decreases the tortuosity, increases the connectivity of pore space, and strengthens the correlation of the voxels in pore space. At the same time, it enhances the surface roughness of the pore space, the proportions of small pores and throats, and the number of isolated pores. Besides, the presence of more OM pores into the pore space leads to the increase of the permeability and decrease of the formation factor of the shale models.

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Inertial Effects on the Pore-scale Capillary Pressure Behavior

Authors: Rabbani Harris [1]; Seers Thomas[1]

[1] *Texas A&M University at Qatar*

Corresponding Authors: thomas.seers@qatar.tamu.edu, harris.rabbani@qatar.tamu.edu

In this research, we reveal the transient behavior of capillary pressure as the fluid-fluid interface travels across the juncture between a converging and uniform capillary, via high-resolution CFD (Computational Fluid Dynamics) simulations. Simulations were performed at different wetting conditions (strong-wet and intermediate-wet) and capillary wall convergence angles. Our results demonstrate that as the angle of convergence increases, capillary pressure at the junction decreases commensurately. Moreover, in contrast to strong-wet conditions, the profile of capillary pressure at the converging-uniform capillary juncture under intermediate-wet conditions is highly non-monotonic, being characterized by a parabola-like form. This non-monotonic behavior is a manifestation of strong inertial forces governing dynamic fluid-fluid interface morphology. This yields conditions that promote the advancement of the fluid-fluid interface, as inertial forces partially nullify the capillary pressure required for the immiscible interface to enter the uniform capillary. In addition to numerical analysis detailed above, a novel theoretical stability criteria that is capable of distinguishing between stable (capillary dominated) and unstable (inertia dominated) interfacial regimes at the converging-uniform capillary juncture is also proposed. In summary, this fundamental study offers new insights into the interface invasion protocol, and paves the way for the re-evaluation of capillary junction controlled interfacial dynamics.

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Research and Application of Numerical Method of Evaluation of Fracturing Effects in Large Scale Volume Reform of Vertical Wells

Author: Debin Xia[1]

Co-authors: Zhengming Yang [2]; Xinlin Zhao ; Wei Lin [1]; Ting Chen [3]; Yutian Luo ; Yapu Zhang ; Anshun Zhang

[1] *Institute of Porous Flow and Fluid Mechanics, Chinese Academy of Sciences, Langfang, Hebei, 065007, P. R. China.*

[2] *PetroChina Research Institute of Petroleum Exploration & Development*

[3] *University of Chinese Academy of Sciences*

Corresponding Authors: zhangyapu69@petrochina.com.cn, 470122295@qq.com, ucaslinwei@126.com, luoyutian@petrochina.com.cn, yzhm69@petrochina.com.cn, chenting15@mails.ucas.edu.cn

The evaluation of the fracturing effect in the tight reservoir with vertical well volume fracturing is usually carried out by direct evaluation methods such as micro-seismic and inclinometer. However, those two methods can only evaluate the fracturing effect at a certain point in time, and they can't effectively evaluate the whole process of the fracturing effect. In this paper, based on the characteristics of seepage flow in the vertical well volume fracturing, we established a two-phase flow numerical method for evaluating the volumetric fracturing effect of vertical wells in tight reservoirs by using mixed meshing technique. At the same time, based on the production data of the two typical conventional fracturing and volume fracturing wells in the Changqing oil field, China, the fracturing effects of the two wells were evaluated. The results suggest that the conventional fracturing only forms a single fracture and can't form the SRV region. After a period of production, the fracture is gradually closed due to the sensitivity of the stratum, and the yield shows an exponential decreasing law. However, the volumetric fracturing transformation can form a complex fracture network system and SRV region, and the yield increase effect is obvious. The effective time lasts for a long time, and the average daily oil increase is 2.2 times that of conventional fracturing. The evaluation method of vertical well fracturing effect established in this study not only realizes the evaluation of the whole fracturing process, but also provides a basis for understanding the vertical well seepage in tight reservoir after fracturing.

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Critical Gas Saturation and Relative Permeability for Pressure Depletion and Gas Injection Processes

Authors: Steffen Berg[1]; Ying Gao[2]; Apostolos Georgiadis[1]; Niels Brussee[1]; Ab Coorn[1]; Hilbert van der Linde[1]; Jesse Dietderich[3]; Faruk Omer Alpak[3]; Daniel Eriksen[1]; Miranda Mooijer-van den Heuvel[1]; Jeff Southwick[1]; Matthias Appel[1]; Ove Bjorn Wilson[1]

[1] *Shell Global Solutions International B.V.*

[2] *Imperial College London*

[3] *Shell International Exploration and Production Inc.*

Corresponding Authors: miranda.mooijer@shell.com, niels.brussee@shell.com, ab.coorn@shell.com, matthias.appel@shell.com, y.gao15@imperial.ac.uk, jeff.southwick@shell.com, o.wilson@shell.com, jesse@metarocklab.com, a.georgiadis@shell.com, omer.alpak@shell.com, d.eriksen@shell.com, steffen.berg@shell.com, hilbert.vanderlinde@shell.com

The critical gas saturation marks the transition from mainly producing oil to mainly producing gas in oil fields that fall during their lifetime below the bubble point. Because of the associated significant technical and economic consequences there is large interest in determining the critical gas saturation in a reliable way. Experimentally measured critical gas saturations range from under 1% to about 50% which gives a very large uncertainty range. The wide range of critical gas saturations observed arises from a complex interaction between phase behavior, pressure decline rate and gas bubble nucleation kinetics.
More importantly, critical gas saturations below 20% are below the percolation threshold which means that the underlying process leading to gas mobility is ultimately not understood. By conducting flow experiments with a model oil-gas system imaged at pore level by X-ray computed microtomography we aim to shed more light on the pore level processes. We find that pressure depletion experiments lead to critical gas saturations consistent with 3D percolation thresholds which does not explain gas mobility below 20% observed in many laboratory studies.
When injecting pure gas near the bubble point we do observe gas mobility below the percolation threshold. The Peclet number < 1 suggests that diffusion leading to compositional gradients coupled with phase behavior effects may lead to the gas mobility below permanent pathways, i.e. below percolation threshold.
These findings suggest that there is a far more complex interplay between flow, diffusive transport and compositional gradients than previously considered. In addition, this methodology can provide at the same time relative permeability computed by lattice Boltzmann simulations based on the imaged fluid distribution which in traditional core flooding experiments is very difficult to obtain.

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Multi-scale iterative scheme for a phase-field model for reactive transport problems.

Author: Manuela Bastidas[1]

Co-authors: Carina Bringedal ; Iuliu Sorin Pop [1]

[1] *Hasselt University*

Corresponding Authors: carina.bringedal@iws.uni-stuttgart.de, sorin.pop@uhasselt.be, manuela.bastidas@uhasselt.be

In a porous medium mineral precipitation and dissolution can significantly alter the pore structure. These reactions affect the porosity and the Darcy-scale flow through the medium. The pore structure changes introduce an evolving boundary between the fluid and grains, and we apply a phase-field approach to model the evolution of the interface.
We consider a two-scale phase-field model of reactive transport processes in porous media. The

model is the result of a formal homogenization procedure where the pore and Darcy scales are coupled through the calculation of effective parameters.
The proposed numerical scheme is a combination of techniques to solve the coupled non-linear system of equations. At each time step, the macro-scale system receives updated information from the cell problems as the phase field evolves. Here we show the maximum principle of the numerical solutions and the convergence of the scheme.
In the numerical examples we combine mesh refinement on the micro scale with different linearization techniques to improve the accuracy and the efficiency of the simulations.

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arXiv preprint arXiv:1903.08717

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Modeling fluid flow/heat/mass transport in an idealized fractal porous structure

Authors: Chenqian Wu[1]; Huijin Xu[1]; Changying Zhao[1]

[1] *Shanghai Jiao Tong University*

Corresponding Authors: xuhuijin@sjtu.edu.cn, wcq23317@sjtu.edu.cn, changying.zhao@sjtu.edu.cn

A new fractal theoretical model with similar morphology to real porous media is established based on the fractal theory. We derived the expression of thermal conductivity, permeability and diffusion coefficient based on the fractal model, which take into account the structural parameters of porous media and fluid properties. The results of the model are compared with the original model data and the results show consistent trend. The results also agree well with the experimental data in literatures, indicating the validity of the study. Effects of the structural parameters and fluid properties on the effective thermal conductivity, permeability and effective diffusion coefficient are compared and analyzed. The effective thermal conductivity, permeability and gas diffusion coefficient of unsaturated porous media with different saturation are provided. The relative permeability of unsaturated porous media is calculated. The effective thermal conductivities under different fluid conditions are compared. The gas-liquid two-phase flow in the condensation process is emphatically analyzed. This study is critical for predicting the fluid flow, the heat and mass transfer performances in porous media and the design of porous structures in related applications.

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The grading evaluation and sweet spot prediction of shale reservoirs based on high-pressure mercury intrusion technology and fractal theory

Author: Yu Zhang[1]

Co-author: Rixin Zhao [1]

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

Corresponding Authors: 17854254903@163.com, zhaorx_damon@qq.com

On the basis of the characterization and classification of the microscopic pore-throat of shale, it is important to establish the lower limit of reservoirs formation and a grading standard of shale oil reservoir, which is crucial for determining the physical sweet spot of shale oil reservoir and favorable target area. Considering that the microscopic throat of shale and its associated pores are the key factors about the quality of shale oil reservoirs, high-pressure mercury intrusion technology combined with fractal theory was used to classify the pore-throat types of shale reservoirs in the northern Songliao Basin and establish reservoir classification evaluation criteria in this study. The results are as follows: According to the inflection points of mercury injection curves and fractal theory, the pore-throats of reservoirs in this study area are divided into four types: microscopic pore-throats (<10nm), small pore-throats (10~50nm), medium pore-throats (50~150nm), and big pore-throats (>150nm), furthermore, based on the number of different types of microscopic pore-throats contained in shale, the reservoirs are divided into I, II and III reservoirs, and their corresponding average pore-throat ranges are Grade I (>75 nm), Grade II (75-40 nm), and Grade III (40-20 nm). The neural network method combined with well logging data was used to predict the porosity, and the shale reservoirs in the study area were graded by the quantitative relationship between porosity and the radius of pore-throats. The shale reservoirs of the Qingshankou Formation in the northern Songliao Basin are better, mainly in the I and II reservoirs, most of them distributed in the southern areas of the Qijia Sag and the Sanzhao Sag; the quality of the shale reservoirs in the Nenjiang Formation is worse compared with the Qingshankou Formation, the reservoirs of Grade II and Grade III are mainly developed, and most of the reservoirs of Grade II are distributed in the southern part of Gulong Sag and the Sanzhao Sag. Comprehensive analysis of reservoir grading characteristics of multiple wells in the study area revealed that the reservoir physical sweet spot in this study area is mainly located in the southern part of the Qijiagulong Sag and Sanzhao Sag.

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How Nanoscale Surface Heterogeneity Impacts Transport of Nano- & Micro-Particles in Granular Media under Environmental Conditions

Author: William Johnson[1]

[1] *University of Utah*

Corresponding Author: william.johnson@utah.edu

Great progress has been made toward providing an underlying theory for transport of nano- and micro-particles (colloids) in environmental granular media, which is needed to support engineering applications ranging from water resource protection to first-tier surface water treatment via riverbank filtration, as well as delivery of novel nanoparticles or bacteria for in-situ subsurface remediation. The distribution of nano- and micro-particles (colloids) with distance from source in granular porous media reflects compounded loss to successive grains encountered along the flow path. However, the resulting distribution from source is well demonstrated to be profoundly influenced by

nanoscale colloid-surface interactions, leading to colloid distributions from source that are exponential when colloid-surface interactions are attractive (so-called favorable for attachment) and that are hyper-exponential or non-monotonic when colloid-surface interactions are repulsive (so-called unfavorable for attachment). The ubiquity of non-exponential colloid distributions from source for all colloid types under unfavorable conditions suggests that nanoscale colloid-surface interactions alter pore scale transport behaviors that in turn alter continuum scale colloid distributions. Impacts are examined of repulsion and inferred nanoscale heterogeneity on pore scale and continuum scale colloid transport behaviors as observed in experiments and as simulated in Lagrangian particle trajectories via mechanistic force/torque balance. The outcomes that link pore- and continuum-scale transport behaviors, and opportunities to parameterize these, are discussed in the context of their propagation to the continuum scale via topological influences from the dual pore and grain network.

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Mechanistic Modelling and Laboratory Evaluation of Immiscible Water-Alternating-Gas Injection and Foam-Assisted Chemical Flooding

Authors: Fabian Torres Mendez[1]; Martijn Janssen[1]

Co-author: Pacelli Zitha [1]

[1] *Delft University of Technology*

Corresponding Authors: p.l.j.zitha@tudelft.nl, m.t.g.janssen@tudelft.nl, fabian.torres.mendez@gmail.com

Recently we have reported an experimental study comparing immiscible gas, water-alternating-gas (WAG) and foam-assisted chemical flooding (FACF) for enhanced oil recovery. We found that oil recovery by FACF is much higher compared to the other gas injection schemes studied, essentially due to the drastic reduction of oil –water interfacial tension (IFT) and good mobility control provided by foam. This paper aims to test and validate proposed mechanisms for the high recovery factor due to FACF, and WAG, by conducting dedicated numerical simulations and by matching numerical simulation results to experimental observations.

1D simulations were conducted using UTCHEM. This comprehensive in-house three-dimensional numerical simulator captures the main features of chemical flooding (geochemistry, phase behaviour, etc.) as well as their coupling with multi-phase flow. CT scan data were used to build models with accurate digital representation of the rock (porosity and permeability). The FACF corefloods were modelled by including the surfactant phase behaviour as a function of salinity, fluid rheology, capillary desaturation of oil, gas mobility reduction to due foam generation, and potential essential geochemical reactions that occurred in the sandstone core.

Relative permeability curves for the primary drainage and water flooding injection stages were determined using the measured saturation distributions by CT scanning in combination with effective permeability measurements based on sectional pressure drops over the core length. History matching WAG injection revealed that gas relative permeability diminished as a function of increasing WAG cycles, which is consistent with gas trapping. Oil mobilization due to injection of a surfactant slug in the FACF experiments, was properly modelled at the two salinity conditions studied. It required successful simulation of the surfactant phase behaviour and obtaining representative relative permeability curves for low IFT flooding. Numerical modelling of drive foam injection, using an alternative local equilibrium approach, resulted in successfully reproducing laboratory observations.

Three-phase diagrams, constructed based on both experimental and numerical modelling results, revealed for the first time which phenomena are dominant for the EOR processes studied. In par-

ticular, the proposed mechanism for oil bank formation and its subsequent displacement by foam during FACF was clearly established.

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Enhanced Gas Recovery evaluated with 1D NMR imaging and relaxometry measurements

Authors: Ming Li[1]; Sarah J. Vogt[1]; Xiaoxian Yang[1]; Paul Connolly[1]; Eric F. May[1]; Michael L. Johns[1]

[1] *University of Western Australia*

Corresponding Author: ming.li@uwa.edu.au

Injection of carbon dioxide (CO2) into a natural gas reservoir is an emerging technology for enhanced natural gas recovery (EGR) realizing increased natural gas production whilst sequestering the injected CO2. However, given that CO2 and natural gas are completely miscible, simulation of potential EGR scenarios is required to determine when breakthrough of CO2 will occur at the natural gas production wells. For such reservoir simulations to be reliable, accurate dispersion data between CO2 and natural gas at relevant reservoir conditions are required. To this end we apply one dimensional (1D) magnetic resonance imaging (MRI) to quantify this dispersion process in-situ in both sandstone and carbonate rock cores. Specifically we apply the SPRITE MRI sequence (Balcom et al. 1996) to facilitate quantitative axial profiles of methane (CH4) content during core flooding processes between CO2 and CH4. Simultaneously we measure, using infrared (IR), the effluent CO2 and CH4 concentrations enabling ex-situ dispersion measurements. Via comparison with the corresponding MRI data, the erroneous contributions to dispersion from entry/exit effects and mixing in piping to and from the rock core holder are quantified. Furthermore, we demonstrate how nuclear magnetic resonance (NMR) T2 measurements can be uniquely used to probe the pore size occupancy of the CH4 during the core flooding process. T2 results suggest that CH4 and CO2 prefer larger pores and smaller pores, respectively, when they coexist in the rock during core flooding. These different pore size occupancies may be related to a relatively high adsorption capability for CO2 on the rock pore surface as compared to that for CH4.

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Identification of Fracture Properties in Shale Oil Reservoirs by a Well Testing Model with"Fracturing-shutting": A Case Study

Authors: Zhiming Chen[1]; Wei Yu[2]; Wendong Wang[3]

[1] *China University of Petroleum at Beijing*

[2] *The University of Texas at Austin*

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

Corresponding Authors: wwdong@upc.edu.cn, zhimingchn@163.com, yuwei127@gmail.com

Fracture networks are of great importance to the management of ground water, carbon sequestration, and petroleum resources in fractured reservoirs. Lots of efforts have been made to investigate the flow regimes with fracture networks. Unfortunately, due to the complexity and arbitrary of fracture networks, it is still a challenge to study the flow regimes in a computationally efficient manner.

Our mesh-free model has the capability to analyze the flow behaviors by considering multi-scale complex fracture networks, non-Darcy flow, and stress dependent permeability of fracture networks. The proposed model includes three domains: (1) matrix with lowest permeability, (2) natural fracture networks with modest permeability, and (3) large-scale fracture networks with highest permeability. Using a dual-continuum approach, we develop the diffusivity equations for gas flow in matrix and natural fracture networks. By applying the nodal analysis technique, we eliminate the flow interplay at fracture intersections and establish the diffusivity equations for flow in large-scale fracture networks. The transient solution of these diffusivity equation is obtained by using Laplace transforms and Stehfest numerical inversion. We verify the proposed model by performing a case study with a numerical simulator for complex fracture networks.

We find that there are about eight flow regimes with multi-scale fracture networks like bilinear flow, formation linear flow, bi-radial flow, transition flow, pseudo-steady state flow, and pseudo-radial flow, etc. Each flow regime has its own special features, which can be used to quantify matrix and fracture properties. For instance, the pseudo boundary-dominated flow provides us the information like how large the area covered by fracture networks. Additionally, we find that the pressure depletion in matrix is smaller with high-conductivity, high-density, large-scale, or high-complexity fracture networks. When compared with the impacts of geometries of fracture networks on pressure depletion, influences of fracture properties are stronger. Furthermore, results indicate that fracture property has the influence on the starting time of some flow regimes. These phenomena offer a possibility to evaluate the properties of fracture networks. What's more, it is found that the non-orthogonal ones have different early flow regimes like bilinear flow, formation linear flow, and pseudo boundary-dominated flow. Based on that, we develop a diagnostic tool to distinguish the non-orthogonal fracture networks from the non-orthogonal ones.

Some reservoirs comprise a huge number of multi-scale complex fracture networks. It is neither practical nor advantageous to use numerical models to analyze the flow behaviors. This paper innovatively develops a mesh-free model for multi-scale complex fracture networks, which provides a throughout understanding of flow behaviors in naturally fractured reservoirs.

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Quantitative Tortuosity Measurements of Carbonate Rocks using Pulsed Field Gradient NMR

Author: Kaishuo Yang[1]

Co-authors: Ming Li [1]; Nicholas N. A. Ling [1]; Eric F. May [1]; Paul R. J. Connolly [1]; Lionel Esteban [2]; Michael B. Clennell [2]; Mohamed Mahmoud [3]; Ammar El-Husseiny [3]; Abdulrauf R. Adebayo [3]; Mahmoud Mohamed Elsayed [3]; Michael L. Johns [1]

[1] *The University of Western Australia*

[2] *CSIRO Energy*

[3] *King Fahd University of Petroleum and Minerals*

Corresponding Authors: ming.li@uwa.edu.au, 22299143@student.uwa.edu.au

Tortuosity is an important physical characteristic of porous materials; for example it is a critical parameter determining the effective diffusion coefficient dictating mixing between miscible fluids in porous rock structures as is relevant to enhanced gas recovery (EGR) processes. Accurate measurement of tortuosity remains challenging, resulting in various definitions dictated largely by the measurement protocol applied. Here we focus primarily on 'diffusive'tortuosity (τd), which is defined as the ratio of the bulk fluid diffusion coefficient to the restricted diffusion coefficient applicable to the porous media under study. Specifically we consider carbonate rock cores ranging in permeability from 2 to 5300 mD, and adapt pulsed field gradient (PFG) NMR methodology such that accurate measurements of tortuosity are obtained over a sufficiently representative length-scale of the porous media. To this end we deploy supercritical methane as a probe molecule exploiting both its high mobility and proton density. Tortuosity measurements are shown to be independent of both pressure and diffusion observation time, conclusively proving that our measurements are in the asymptotic regime in which all of the pore space is adequately sampled by the diffusing methane molecules. The resultant 'diffusive'tortuosity measurements (which ranged from 3.1-5.6) are then compared against independent electrical conductivity measurements of tortuosity using a two-electrode impedance technique applied to the carbonate samples saturated with brine solution. Agreement between the 'diffusive tortuosity', as measured by PFG NMR, and 'electrical'tortuosity was remarkably good (within 10%), given the very different measurements techniques used, for most of the carbonate rock samples considered.

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Pipe Network Modelling for Fractured Rock Cores with Micro-computed Tomography Imaging

Authors: YU JING[None]; Ryan Armstrong[None]; Peyman Mostaghimi[None]

Corresponding Authors: yu.jing@unsw.edu.au, peyman@unsw.edu.au, ryan.armstrong@unsw.edu.au

The fracture network plays a critical role in controlling flow pathways of fractured rock. The study of deep fractured rocks has a wide range of applications, such as groundwater management (Wellman, Shapiro, & Hill, 2009), oil and gas developments (Mostaghimi et al., 2017), CO2 storage (Zhang, Lebedev, Jing, Yu, & Iglauer, 2019), geothermal extraction (Pruess, 1983), and nuclear waste disposal (Seetharam, Perko, Jacques, & Mallants, 2014). Therefore, the characterisation of fracture system and fluid flow analysis for fractured rock are becoming increasingly important. To characterise fracture systems, X-ray micro-computed tomography imaging (micro-CT) has been widely applied as it enables us to visualise the internal fracture network in 3D. The obtained high-quality 3D digital images of the fracture network are then utilised to derive petrophysical properties of the network by performing flow simulations. One method of obtaining petrophysical properties is to perform numerical simulation directly on the micro-CT images (Mostaghimi, Blunt, & Bijeljic, 2013). Despite that the direct simulation methods are precise, they are extremely computational demanding because of the large image data.

Therefore, to reduce the high computational cost, a common method is to simplify the fracture network into one-dimensional pipe network approximations, which is called Pipe Network Model (PNM). In this work, we construct PNM based on 3D micro-CT images of fractured coal samples to efficiently estimate the permeability of coal fractured network. To analyse the fracture connectivity,

deterministic Discrete Fracture Network (DFN) models are firstly constructed where fracture geometrical properties (eg. fracture centres, orientations, lengths and aperture sizes) are measured from micro-CT images. Integrated with DFN models, PNM models are created, where pipe conductivity are determined by real fractures in micro-CT images and pipe connectivity is obtained from DFN models.

By comparing permeability values obtained from PNMs and values from micro-CT images and voxelised DFNs, we conclude that PNM modelling can effectively estimate the permeability of original fracture networks, most importantly, requiring significantly less computational cost. Apart from permeability, pressure fields can also be obtained quickly. Pore pressure is a paramount parameter in some engineering fields. For example, as the pore pressure decrease in coal seam gas (CSG) reservoirs, methane starts to desorb from coal matrix and flows through fractures to production. In addition to the advantage of computational efficiency, PNM is more preferable for the challenging multi-phase flow simulation.

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Dynamic hydraulic fracturing in naturally fractured reservoirs

Authors: Mohammad Vahab[1]; Mohammadreza Hirmand[2]; Nasser Khalili[3]

[1] *UNSW Australia*

[2] *University of Waterloo*

[3] *UNSW*

Corresponding Author: m.vahab@unsw.edu.au

We propose an energy based hydro-mechanical model and computational algorithm for the problem of hydraulically driven fracture networks developing in naturally fractured impermeable media. The proposed model is based on non-differentiable energy minimization for the dynamic deformation and fracture of the body coupled with mass balance of fluid flow within the hydro-fractures. We show that the use of a time-continuous fracture model, such as the present non-differentiable energy minimization model, is crucial for the numerical soundness and stability of the hydraulic fracture propagation algorithm. The reason is that time-discontinuous models give rise to spurious crack opening velocity fields which lead to unphysical solutions for the coupled fluid pressure field defined locally along the crack faces. A discontinuous Galerkin finite element formulation is implemented, in which every element edge in the mesh is a potential site of hydro-fracture initiation and propagation. Pre-existing natural fractures can be modelled with desirable flexibility by simply assigning different

fracture properties to the element edges defining the natural fractures. Because the method allows for activation of cracks away from the evolving hydro-fracture, a search algorithm is proposed to identify the sub-set of cracked interfaces that form the domain on which the mass balance equation is defined and solved. Robustness of the proposed computational algorithm and its versatility in the study of hydraulic fracturing is shown by presenting several numerical simulations.

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Dynamic of ice lens formation in frozen soil

Authors: Signe Kjelstrup[1]; Seyed Ali Ghoreishian Amiri[2]; Hao Gao[2]; Gustav Grimstad[2]; Benoit Loranger[3]

[1] *PoreLab, Department of Chemistry, Norwegian University of Science and Technology*

[2] *PoreLab, Department of Civil and Environmental Engineering, Norwegian University of Science and Technology,*

[3] *Department of Civil and Environmental Engineering, Norwegian University of Science and Technology,*

Corresponding Authors: signe.kjelstrup@ntnu.no, hao.gao@ntnu.no, benoit.loranger@ntnu.no, seyed.amiri@ntnu.no, gustav.grimstad@ntnu.no

Soil freezing can be associated with a very destructive phenomenon called frost heave. It is defined as the upward movement of the ground surface due to formation of ice lenses within the fine-grained soil. The phenomenon is related to transport of sub-cooled water towards the frozen fringe which potentially can form thick ice lenses. Experimental studies (e.g. [1]) showed that this water transport is proportional to the temperature gradient across the frozen fringe. Assuming a constant proportionality factor(known as segregation potential), Konrad and Morgenstern [2] constructed an engineering theory of frost heave.
Using non-equilibrium thermodynamics, Førland and Kjelstrup Ratkje [3] theoretically described this coupled transportation phenomenon. They showed that in frozen soil, flow of mass and heat are strongly coupled to each other. Three transport coefficients are enough to model the process: the hydraulic and thermal conductivity, and what we name the "frost heave coefficient". In fact, the frost heave coefficient and the segregation potential, defined by Konrad and Morgenstern [2], are basically the same. However, we have shown that this coefficient is not constant, but it is a function of unfrozen water content. This dependency is very important, since it is governing the growing rate of the ice lens, and potentially defines criteria to stop its growth in case of temperature drops.
Indeed, in the engineering theory of frost heave, the segregation potential is defined as an independent parameter, which should be evaluated from a one-dimensional frost heave experiment, when the thermal regime of the specimen switches from transient to steady-state condition. On the contrary, we have shown that the frost heave coefficient includes the hydraulic conductivity.
The coupled transport equations for mass and heat, together with the mass balance and energy balance equations, are generally enough to describe the growth of a single ice lens in a predefined position, but they cannot describe the dynamics of the system and predict formation of multiple ice lenses and their positions. To complete the set of equations so as to describe the dynamics of the system, the momentum balance equation must be added. This controls the deformation of the frozen soil skeleton, and has been taken into account in the present study. Fracture mechanics is indeed employed to predict the position of the ice lenses.

Acknowledgments

This work is supported by the Research council of Norway through its Centers of Excellence funding Scheme, project number 262644.

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Sensitivity Analysis on Different Parameters Affecting the Gas-Oil Gravity Drainage Mechanism in Naturally Fractured Reservoirs

Authors: Mohammad Madani[1]; Amin Daryasafar[2]

[1] *Amirkabir University of Technology*

[2] *Petroleum University of Technology*

Corresponding Authors: amindaryasafar@yahoo.com, m_madani70@yahoo.com

In fractured reservoirs with primary gas cap, the gas, having high mobility, moves faster than oil and consequently forms a new zone above the oil zone. In this zone, which is named gas invaded zone, gas-oil gravity drainage (GOGD) is the major mechanism contributing to oil recovery. The prediction of GOGD performance is highly dependent on capillary continuity and reinfiltration phenomena. Therefore, studying various parameters related to these phenomena is crucial. To evaluate the effect of capillary and reinfiltration on gravity drainage mechanism, a fractured porous medium was modeled using a commercial simulator, ECLIPSE-100. The impact of different parameters such as matrix block height, fracture and matrix permeabilities, fracture width, fracture and matrix capillary pressure, initial water saturation, different percentages (0%, 16%, 32%, 36% and 100%) and patterns of capillary continuity between blocks, system with different rock types and also oils with various PVT properties on the performance of GOGD in producing oil is investigated in this study. In addition, foam injection, as an enhanced oil recovery technique, is used for improving oil recovery in gas invaded zone and its effect on both oil recovery efficiency and oil flow rate is demonstrated by numerical simulation. The base-case simulation runs showed that about 38.5% of the original oil in-place (OOIP) in the porous media could be recovered by GOGD mechanism. Furthermore, the sensitivity analysis with the aid of simulation runs demonstrated that among various parameters, existence of capillary continuity, matrix capillary pressure, initial water saturation, and matrix block height have the most significant influence on ultimate recovery, while fracture width has no effect on GOGD performance. Also, matrix permeability could significantly affect the produced oil flow rate. The results of foam flooding in gas invaded zone illustrated that it is so important for a reservoir to be flooded by foam in the early years of production since it can enhance the performance of GOGD and improve oil production.

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Capillary instabilities during two-phase flow process in a porous medium

Authors: Tao Zhang[1]; Rui Wu[1]

[1] *Shanghai Jiao Tong University*

Corresponding Authors: 1448695561@sjtu.edu.cn, ruiwu@sjtu.edu.cn

Two-phase flow process in porous media is ubiquitous in nature and many industrial applications, such as in petroleum engineering (oil and gas recovery), remediation of contaminated soils by vapor extraction, water management of proton exchange membrane fuel cells, and pharmaceutical industries. Two-phase flow process in porous media is widely accepted as quasi-static (capillary-dominated) or viscous-dominated process. However, in our microfluidic experiments based on a pore network consists of large pore bodies connected by small pore throats, we found that even during slow evaporation in porous media, a fast dynamics, i.e. capillary instabilities, induced by interaction between different gas-liquid interfaces can happen, whose time scale is much smaller than the time scale of slow evaporation process. In the capillary instabilities, the phase distribution in the pore network can be changed rapidly compare to the evaporation process, and the phase distribution to a great extent can determine the evaporation process in porous media. Therefore, the capillary instabilities should be researched for better understanding of evaporation process in porous media. Moreover, during the initial stage of imbibition into a porous media and other immiscible displacement in porous media, numerous dynamics exist, but which cannot be well described by traditional theories. Furthermore, the rapid dynamics means the existence of inertial effects during two-phase flow in a porous media, but which is hardly considered by previous studies. More interestingly, the capillary instabilities are also influenced by some pore-scale mechanisms. In our experiments using microscope, we found that the existence of residual wetting liquid in a pore body and the corner liquid film may reduce the threshold pressure of the wetting liquid refilling into the pore body, which in turn intensifies the capillary instabilities. In addition, the number of pore throats occupied by wetting liquid adjacent to a pore body partially occupied by wetting liquid also determines the pressure needed to invade the pore body. In order to analyze the effects of inertial forces and pore-scale mechanisms on two-phase flow in a porous media, a pore network model that considers capillary forces, viscous forces, inertial forces and pore-scale mechanisms is built and the numerical results obtained from the model compare well with experimental results. These analyses based on experiments and model further enrich our understanding of two-phase flow in porous media.

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Experimental analysis of plumes transport and dilution processes under highly transient boundary conditions

Author: Mónica Basilio Hazas[1]

Co-authors: Francesca Ziliotto [1]; Massimo Rolle [2]; Gabriele Chiogna [1]

[1] *Technical University of Munich*

[2] *Technical University of Denmark*

Corresponding Authors: masro@env.dtu.dk, ga53zaw@mytum.de, gabriele.chiogna@tum.de, monica.basilio@tum.de

The boundary conditions and the heterogeneity of the porous media play an important role in the fate and transport of dissolved solutes and contaminants in the subsurface. Transient boundary conditions can affect the groundwater flow field and the mixing and mixing-controlled degradation of contaminants. In this study, we investigate at laboratory scale the effect of highly transient boundary conditions on groundwater flow and transport in porous media. We design and perform flow-through experiments inspired by a practical hydrologic problem: hydropeaking, an artificial river regime caused by the operation of hydropower plants. The setup consists of a quasi-two-dimensional flow-through chamber filled with a porous medium and mimicking a shallow unconfined aquifer in

hydraulic contact with two rivers connected to two different water reservoirs. Changes in the height of the reservoirs emulate changes in the river stage and generate transient groundwater flow fields. We injected a color tracer to compare the evolution of a plume under steady state and transient boundary conditions. Sampling at the outlet and non-invasive visualization techniques allowed us to map the concentrations of the tracer during the whole experiment. We investigated the behavior of the plume under steady-state and transient groundwater flows by analyzing the concentration breakthrough curves measured at the outlet, as well as the evolution of plume spreading and mixing. We complemented our analysis with flow and transport simulations that helped the quantitative interpretation of the experimental observations.

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A vertically integrated approach to field-scale modelling of mineral trapping in reactive rocks

Authors: Tom Postma[1]; Karl Bandilla[1]; Mike Celia[None]

[1] *Princeton University*

Corresponding Authors: celia@princeton.edu, tpostma@princeton.edu, bandilla@princeton.edu

Mineral trapping of CO_2 is the most stable of all trapping mechanisms identified in carbon capture and storage (CCS). However, in most sedimentary formations, the time scales on which significant mineral trapping occurs are too large for it to be of practical significance (Gilfillan et al., 2009; Matter and Kelemen, 2009).

Conversely, flood basalts, a category of igneous rock formations with a distinctive mineralogy, have the potential for relatively rapid mineral trapping. This occurs via dissolution of basaltic minerals and subsequent precipitation of carbonates, both of which can happen over short time scales (McGrail et al., 2006). Use of basalt formations for CO_2 storage has been studied in different ways, including small-scale pilot projects in Iceland and the United States that showed promising results (McGrail et al., 2017; Matter et al., 2016).

As minerals continuously dissolve and precipitate, the rock matrix forms a dynamic part of the system, with rock properties expected to change over time as a function of dissolution and precipitation. Such changes to rock properties may have important consequences for the viability of full scale CCS projects. This is especially true for injection scenarios that may have fluctuations in injection rates, including intermittent stops. The resulting system of different coupled processes occurring on various spatial and temporal scales, combined with the uncertainties inherent in modelling the subsurface, calls for a flexible and efficient simulation tool.

Currently, numerical simulations of reactive transport in the subsurface rely on computationally expensive methods, which resolve the domain in all three spatial dimensions and track virtually all possible reactions that may occur (see e.g. Aradóttir et al. (2012) and Bacon et al. (2014)). These methods quickly become prohibitively expensive for field-scale models, especially when considering complex injection schedules with extensive post-injection periods during which the stored CO_2 is immobilized.

The present work develops a computationally efficient vertically-averaged approach to field-scale modelling of mineral trapping in reactive rocks. We use a splitting-type approach, alternately solving for component transport and chemistry, allowing for flexibility in the exact description and modelling approach used for either.

Building on the work of Gasda et al. (2009), we solve the two-phase flow problem under the assumption of vertical equilibrium with respect to fluid flow. This allows for vertical integration of the

governing equations, reducing the number of spatial dimensions by one. Dissolution of CO_2 into the brine phase, including convection-driven dissolution into the brine column, is incorporated.

Further assuming a negligibly small capillary fringe, we distinguish three zones in the domain:the mobile CO_2 plume, a region of CO_2 at irreducible saturation, and a region fully saturated with brine. At each horizontal location in the domain, we solve for the chemical reactions in each of these three zones, assuming the chemical composition is homogeneous in each of them.The proposed method provides a significant reduction in computational cost, enabling efficient reservoir simulation for CCS in reactive rocks.

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Analysis of Low Resistivity of Gravel Sandstone Reservoir in Beibuwan Basin Based on Petrophysical Experiments

Authors: Weichao Yan[None]; Jianmeng Sun[1]; Likai Cui[2]

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

[2] *Northeast Petroleum University*

Corresponding Authors: cui_lk@nepu.edu.cn, sunjm@upc.edu.cn, yanweichaoqz@163.com

The pore structure of gravel-bearing sandstone reservoirs in Beibuwan Basin is complex and changeable, and the variation law of reservoir resistivity is very complex. The resistivity of some pure oil layers is lower than that of mudstone or water layers, which is contrary to the understanding of

the conductivity law of conventional oil layers, and the oil-water layers tested by some interpretations come out together, which makes it difficult to identify oil-water layers and the cause of low resistivity of reservoirs. As well as the unclear understanding of conductive mechanism, it seriously restricts the fluid identification and fine evaluation in the subsequent exploration and development of such reservoirs in Beibuwan Basin. This paper clarifies the conductive mechanism of conglomerate-bearing sandstone reservoirs in Beibuwan Basin by means of more than ten advanced experimental techniques, such as conventional core experiment method and CT scanning digital core method, and carries out the calibration of digital core simulation results by using actual core experiment results, and systematically explores the genesis mechanism of low resistivity through experimental and simulation studies. During the experiment, dual-mode scanning (nano-scale mineral distribution imaging and surface structure imaging) was used for the first time to analyze minerals inside and outside the pore, and micro-pore was found in feldspar, illite and other minerals; full-pore and full-component three-dimensional digital core was constructed to carry out formation water salinity, mud in the pore, micro-pore, water film thickness and other factors. Finally, it is concluded that the main cause of low resistivity reservoir in this area is the development of micropore, and the salinity of high formation water is also an important cause of low resistivity.

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Investigations of pore connectivities and permeabilities of fractured vuggy carbonates based on digital rock techniques

Authors: Weichao Yan[None]; Sun Jianmeng[1]

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

Corresponding Authors: sunjm@upc.edu.cn, yanweichaoqz@163.com

Deep carbonate reservoirs of Sinian-Cambrian System in Gaoshiti-Moxi block of Sichuan Basin belong to ancient hilly beach reservoirs, which has the characteristics of deep burial, low porosity and permeability, development of fracture and vug, and strong heterogeneity, that makes it difficult to evaluate the reservoir permeability by logging method. The diversity of reservoir space, dissolution and fracture lead to complex pore structure, that bring challenges to reservoir connectivity analysis and effectiveness evaluation. Various coupling forms of pore, hole and fracture make the reservoir highly heterogeneous, and the pore-permeability relationship is not obvious due to the development of cracks, that make it difficult to calculate reservoir parameters. According to the reservoir characteristics in the study area, through digital core experiments and matching rock physics experiments, the research on reservoir connectivity analysis and permeability modeling technology is carried out. The connectivity is mainly determined by the connection mode and efficiency of macropore, mesopore and micropore. The calculation model of reservoir permeability logging is established, which effectively solves the technical problem of multi-medium reservoir permeability logging evaluation and improves the accuracy and reliability of reservoir logging interpretation and evaluation in the study area.

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Estimation of Subsurface Hydraulic Conductivities using Geophysical Signatures

Authors: Debasmita Misra[1]; Peter Calvin[2]

[1] *University of Alaska Fairbanks*

[2] *CLEAResult*

Corresponding Authors: peter.calvin@gmail.com, dmisra@alaska.edu

The objective of this research was to explore a cost-effective and non-invasive methodology to characterize spatial variability of hydraulic conductivity using airborne electromagnetic (AEM) signatures as an alternative to traditional techniques such as borehole sampling. The relationship of AEM measured apparent resistivity and magnetic field strength was explored using a small dataset that included 180 natural moisture (NM) content data and a total dataset of 546 grain size distributions that excluded the NM. The grain size distributions were used to develop soil indicator parameter and to estimate the hydraulic conductivity (K*) using pedo-transfer functions. Predictive models were developed using three techniques; artificial neural network regression (ANNR), support vector regression (SVR), and artificial neural network classification (ANNC). The sole use of non-invasive parameters to characterize K* proved insufficient. The inclusion of supplemental invasively collected parameters showed ANNR to best characterize the relationship (R2 = 0.64) with the smaller dataset; while SVR model performed best with the total dataset (R2 = 0.57). ANNC was shown to be a viable alternative (overall accuracy = 88%) when broad characterization of K*was sufficient. This study lays out a methodology that could be used for future K* characterization using improved data set.

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Numerical and semi-analytical investigation on forced convection in tubes fully/partially filled with metal foams

Author: Farshid Jamshidi[1]

Co-authors: Anastasia August [2]; Andreas Reiter [1]; Aron Kneer [3]; Michael Selzer [2]; Britta Nestler [2]

[1] *Karlsruhe University of Applied Sciences*

[2] *Karlsruhe Institute of Technology*

[3] *TinniT Technologies GmbH*

Corresponding Authors: a.kneer@tinnit.de, andreas.reiter@partner.kit.edu, michael.selzer@kit.edu, farshid.jamshidi@hs-karlsruhe.de, anastasia.august2@kit.edu, britta.nestler@kit.edu

In this work, we study open-pored metal foams that can be used in a variety of applications. This is because they are lightweight, they have a high specific surface area as well as high thermal conductivity and also outstanding capability in flow mixing. These characteristics make the foams very popular for heat transfer applications such as heat exchangers where the foams are placed inside the pipes and the pipes are inductively heated up. This enhanced heat transfer helps to reduce the NO_x emission of modern condensing boilers that are fuelled by oil or gas. Moreover, it can be a more efficient and resource-saving method of heat transfer if the design criteria of the porous structures inside the pipes such as improved wetting rate and lower pressure loss are considered.

By Computational Fluid Dynamics (CFD) simulations as well as a developed semi-analytical model, these design criteria are studied in pipes that are fully filled with open-pored metal foams as well as pipes with a foam-free region. For CFD simulations, an in-house package named PACE3D based

on the numerical solution of the Navier-Stokes and the heat conduction/convection transport equations is used. Further, for the semi-analytical model, the Brinkman-extended Darcy and the local thermal non-equilibrium equations are implemented. To validate the simulation/model results, we compare them with experimental data available in the literature and we find reasonably good agreement particularly for high porosity foams with high thermal conductivity and low flow Reynolds numbers.

The optimization focuses on the velocity and temperature profiles in the pipes; to understand how the pressure drop and the Nusselt number depend on parameters such as the flow Reynolds number, the porosity of the foam, the radius of the foam-free region and the ratio of thermal conductivity of the fluid to that of the solid. For the structures inserted in the pipe, we examine different open-pored foams, which are generated using a modified Voronoi tessellation algorithm. As expected, by decreasing the porosity, the flow Reynolds number increases and the heat transfer enhances, however, the pressure loss increases. By choosing metal with higher thermal conductivity as the material of the foam, the Nusselt number rises without causing any major hydraulic losses. The presence of non-porous areas in the pipe center or graded porosities is another solution to this problem.

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Visualization of CH4 Hydrate Dissociation Under Permafrost Temperature Conditions Using High-Pressure Micromodel

Author: Jyoti Shanker Pandey[1]

Co-authors: Stian Almenningen [2]; Nicolas von Solms [1]; Geir Ersland [2]

[1] *Technical University of Denmark*

[2] *University of Bergen*

Corresponding Authors: geir.ersland@uib.no, nvs@kt.dtu.dk, stian.almenningen@uib.no, jyshp@kt.dtu.dk

Methane (CH4) gas hydrate formation, dissociation, and stability in permafrost sediments are essential to model these systems concerning global warming and in schemes of CH4 recovery and/or carbon dioxide (CO2) storage. It is known that CH4 hydrate is thermodynamically less stable than CO2 hydrate due to the lower activation energy of the decomposition. However, recent studies show that CH4 hydrate's dissociation slows down in subzero temperature due to the self-preservation mechanism. Thus, a fundamental understanding of CH4 hydrate distribution, dissociation mechanism, and self-preservation in sediments at the pore-scale level, is essential to optimize the CH4 gas production method from permafrost-affected hydrate reservoirs.

In this study, CH4 hydrate dissociation was visualized using a high-pressure, water-wet, silicon-wafer based micromodel with pore network of actual sandstone rock. A total of nine runs were performed, and CH4 hydrate was formed between 60-85 bar, and between 273.15 K-275 K. CH4 hydrate was dissociated between 270-275K by pressure depletion to evaluate the effect of hydrate and fluid saturation on dissociation rate, self-preservation, and risk of hydrate reformation. Below 273.15K, the CH4 gas production was limited due to rapid formation of ice from liquid water liberated from initial hydrate dissociation. The liberated CH4 gas was immobilized and trapped by the formed ice. Consequently, we demonstrate the ineffectiveness of depressurizing CH4 hydrate without thermal stimulation. The results highlight the importance of initial hydrate/ice/gas saturations and free gas availability in characterizing hydrate dissociation patterns.

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Tracing back the source of contamination

Authors: J. Jaime Gómez-Hernández[1]; Zi Chen[1]; Andrea Zanini[2]

[1] *Institute for Water and Environmental Engineering, Universitat Politècnica de València*

[2] *Università di Parma*

Corresponding Authors: andrea.zanini@unipr.it, dtpenguincz@gmail.com, jgomez@upv.es

From the time a contaminant is detected in an observation well, the question of where and when the contaminant was introduced in the aquifer needs an answer. Many techniques have been proposed to answer this question, but virtually all of them assume that the aquifer and its dynamics are perfectly known. This work discusses a new approach for the simultaneous identification of the contaminant source location and the spatial variability of hydraulic conductivity in an aquifer which has been validated on synthetic and laboratory experiments and which is in the process of being validated on a real aquifer.

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Flow Law of Foam in Fractured Vuggy Reservoir

Author: Zhengxiao Xu[1]

Co-authors: Zhaomin Li [1]; Binfei Li [1]; Longkun Chen [1]; Danqi Chen [1]; Zihan Gu [1]

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

Corresponding Authors: lizhm@upc.edu.cn, b18020040@s.upc.edu.cn, cdq0813@163.com, chenlk_1994@foxmail.com, 1113606439@qq.com, libinfei999@126.com

There are many types of carbonate reservoir in China. Most of the gas reservoirs are porous media, while the oil reservoirs are mostly fracture-pore and fracture-cavity media. The fluid is characterized by a variety of flow patterns, with large caves and slits being dominated by free flow, and small scale spaces dominated by seepage. The development features are quite different, and the foam is often used for flow-blocking.
In view of the flow characteristics of foam in fractured vuggy reservoir, a variety of visual fracture models were designed. Foam morphology and foam flow path under different flow conditions were observed, the flow resistance under different foam quality and flow rates was tested. The results show that in the visual fracture models, different crack opening changes the microstructure of the foam and affects the flow characteristics. As the crack opening increases, the liquid film thickness of the foam decreases, the particle size increases, and the migration velocity slows down. The injection of foam leads to increased flow resistance in high permeability fractures and helps to transfer injected fluid to low permeability regions. Under the same injection gas / liquid ratio, the flow resistance of the foam increases with the increase of flow rate. At the same injection rate, the flow resistance of the foam increases first and then decreases with the increase of the foam quality, and reaches a maximum within the range of the foam quality of 90%-92%. This study is conducive to summarize the flow law of foam in the fracture network and to achieve efficient development of carbonate reservoirs.

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Lattice Boltzmann simulation of amphiphilic fluids flow through porous media

Author: Bei Wei[1]

Co-authors: Jian Hou [1]; Michael Sukop [2]

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

[2] *Florida International University*

Corresponding Author: bwei@vip.163.com

We establish a surfactant Lattice Boltzmann (LB) method and show the applications in porous media in this work.
The numerical simulation method is established as follows. We firstly introduces an active solute component, i.e., the surfactant into the pseudopotential multiphase LB model, so that the transport of surfactants follows the convection-diffusion equation macroscopically. Then we characterize the amphiphilic structure of surfactants using a dipole equivalent model, in which the interactions related with surfactants depend not only on particle relative distances but also on their dipolar orientations. By this way, it successfully captures the effect of interfacial tension (IFT) reduction resulting from the surfactants aggregation at the interface. Moreover, we consider the surfactants adsorption onto the solid walls by adding a surfactant-solid interactive force. As surfactants on the solid surface will alter the wettability, we further give a wettability alteration (including wettability reversal) scheme for the model. The surfactant LB method is verified by comparing the droplet deformation results with the level set method.
We investigate three problems use the established model, i.e., droplet detachment from the wall, emulsions flow in constricted capillaries, and surfactant-enhanced aquifer remediation (SEAR) process. The simulation results show that surfactants decrease the adhesion work on walls by IFT reduction and wettability reversal, and can reduce the critical Bond number for oil detaching from walls by up to 90%. When emulsions flow through a constricted capillary, the presence of surfactants can change the shape of small droplets in the confined throat, help large droplets overcome the Jamin effect, influence the oil configuration by wettability alteration, inhibit the droplet coalescence, and prohibit the snap-off phenomenon. Moreover, oil recovery is improved with the presence of surfactants in SEAR, but it does not mean the more surfactants the better, because adsorption onto walls leads to unnecessary waste and could decrease the surfactant concentration in the bulk phase.
In brief, the model provides a powerful tool to simulate the amphiphilic fluids flow at pore scale. Especially, it has great advantage in simulating flows in porous media for it is a "bottom-up"method and can handle complex solid wall boundaries efficiently.

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Water transport in a gas diffusion layer of polymer electrolyte fuel cells in the presence of polytetrafluorethylene

Authors: Dieter Froning[1]; Uwe Reimer[1]; Werner Lehnert[1]

[1] *Forschungszentrum Jülich GmbH, Germany*

Corresponding Authors: w.lehnert@fz-juelich.de, d.froning@fz-juelich.de, u.reimer@fz-juelich.de

In polymer electrolyte fuel cells (PEFCs), the transport of liquid water is highly relevant for the efficient operation of the stack. The water is produced on the cathode side and must be transported through the thin porous structure of the gas diffusion layer (GDL). This medium is typically made of carbon fibers, and for hydrophobicity is often treated with polytetrafluorethylene (PTPE). The total amount of PTFE in the thin layer is specified by the manufacturer, but the local distribution is usually not known. On the other hand, it is known that the PTFE distribution on the outer surfaces and inside the GDL is not homogeneous [1].

In this work, the impact of PTFE distribution inside the GDL on transport properties will be discussed. In earlier work, the random nature of fiber localizations was discussed [2, 3]. The distribution of PTFE is another stochastic element that can influence water transport. The first results on the impact of the PTFE distribution were presented by Yu et al. [4] and still use a simplified assumption of the local distribution of PTFE across the fibers. On the other hand, local preferences of PTFE accumulation have already been observed by Daino and Kandlikar [5], while Rofaiel et al. [6] found inhomogeneities in the global distribution of PTFE.
In this work, a more detailed view on PTFE distribution is given. The local accumulation of PTFE near fiber crossings is considered, as well as the global accumulation of PTFE in certain regions of the GDL.

Water transport in GDLs is based on micro-structures created by a stochastic geometry model [7] and transferred to Lattice Boltzmann (LB) simulations via a series of binary images. One color (white) represents the void space, while the other (black) represents the solid fraction. The hydrophobicity of the solid material can be specified by a local contact angle. PTFE can be applied randomly to the geometry representation by introducing three-colored images, the third color specifying positions where the fibers are hydrophobic because of being covered by PTFE. In this presentation, previous work presented by Yu et al. [4] is continued by analyzing the macroscopic impact of PTFE on water transport from a statistical viewpoint.

Transport simulations are running on the hardware of the Jülich Supercomputing Centre, grant CJIEK30.

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Dynamic Multilevel Simulation of Coupled Flow-Heat Transport in Fractured Porous Media

Author: Mousa HosseiniMehr[1]

Co-authors: Cornelis Vuik [1]; Hadi Hajibeygi [1]

[1] *TU Delft*

Corresponding Authors: h.hajibeygi@tudelft.nl, s.hosseinimehr@tudelft.nl, c.vuik@tudelft.nl

In various geo-engineering applications, accurate, efficient and scalable modeling of coupled fluid-heat transport in fractured porous media is of paramount importance. However, achieving such task faces several geological, physical and computational key challenges. Demand for high-resolution computational grids, non-linear behavior of the system due to strong mass-heat coupling and presence of fractures (or faults) with wide heterogeneity contrasts are few among many to mention.

In this work, an algebraic dynamic multilevel method for simulation of coupled flow-heat transport in fractured porous media with projection-based Embedded Discrete Fracture Model (pEDFM) is devised. The proposed method provides a scalable and efficient simulation framework for large and real-field scale heterogeneous fractured reservoirs.

pEDFM formulation is extended to account for generic 3D fracture geometries, providing a consistent formulation approach to capture complex flow physics in presence of explicit fractures which can act from highly conductive manifolds to flow barriers. Within a robust fully-implicit scheme, the fine-scale system is mapped into a dynamically defined multilevel grid resolution system via a front tracking technique by detecting the sharp gradients of solution at previous time-steps (set by a user-defined threshold). Such automatic determination of resolution results in significant error reduction and higher accuracy. To obtain this map (i.e., ADM map) multilevel multiscale coarse grids are constructed for matrix as well as each fracture at all coarsening levels. Sequences of restriction and prolongation operators are developed to generate an accurate map between fine-scale and hierarchical multilevel multiscale systems to honor fine-scale heterogeneities. Local mass is conserved across all resolutions by using finite-volume restriction operators. The prolongation operators are built by obtaining basis functions at all coarsening levels. Once the system is solved at ADM level, the solution is prolonged back to fine-scale resolution.

The performance of our method is studied for a range of 2D and 3D test cases including fractures with higher and lower conductivities compared with that of the matrix. It is shown that our method provides accurate and scalable simulation framework for highly fractured heterogeneous reservoirs. Importantly, we study the sensitivity of the production estimations with respect to the fracture density, orientation and properties. In addition, the scalability of the simulation approach for large-scale geo-models is discussed. Our results demonstrate that the proposed method is capable of simulating large-scale fractured reservoir models.

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Quantitative evaluation of mobile shale oil at different pore sizes

Authors: Ning Qi[None]; Mingyue Lu[None]; Haitao Xue[None]; Jinxiu Yang[None]; Bojie Zhang[None]; Dongquan Sun[None]; Xueping Liu[None]; Jiafan Tang[None]

Corresponding Authors: 1127888260@qq.com, 676751466@qq.com, 747917094@qq.com, 49142456@qq.com, 290911353@qq.com, 2976005137@qq.com, 496161706@qq.com, 1430067486@qq.com

With the consumption of conventional hydrocarbon resources, the successful exploration and development of unconventional petroleum has largely alleviated the contradiction of global oil and gas supply and consumption. Continental shale oil resources have great potential in China, which is an ideal replacement field of oil and gas resources in the future. In recent years, researches on shale oil reservoirs have attracted the attention of scholars at home and abroad, and detailed studies have been carried out on the characteristics of shale reservoirs and the occurrence state of shale oil, but relatively few studies have been conducted on the mobility of shale oil at different scales.
Therefore, we selected typical continental shale samples from sedimentary basin in eastern China to conduct low-temperature nitrogen adsorption (LTNA), high-pressure mercury injection (HPMI) and nuclear magnetic resonance (NMR) to quantitatively reveal the distribution characteristics of movable shale oil at different pore scales. Based on the pore diameter distribution curve of LTNA, the T2 spectrum distribution curve in the time domain of NMR was calibrated as the pore diameter distribution curve in the length domain. Reservoir spaces of the shale oil reservoir were further divided into micropores (<10nm), small pores (10-100nm), mesopores (100-1000nm) and macropores (>1000nm), according to the fractal features of high-pressure mercury injection curve and mercury inlet characteristics. On the basis of the NMR pore diameter distribution curve of shale samples at different centrifugal speeds (Figure 1), the proportion of movable oil in selected shale samples was 54%, among which, the proportion of movable oil in large, medium, small and micro pores was 64%, 52%, 11% and 5%, respectively. Generally, large pores and mesopores contribute the most to fluid mobility in the reservoir, followed by small pores, and micropores have little contribution to fluid mobility in the reservoir, among which liquid hydrocarbon mainly exists in adsorption state. Shale reservoirs with abundant large-medium pores (>100nm) are the "sweet spot" for shale oil exploration and development.

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Influence Mechanism of Potential Determining Ions on Oil-in-water Emulsion Stability in Smart Water-flooding

Authors: Rukuan CHAI[1]; Yuetian LIU[1]; Liang XUE[1]

[1] *State key Laboratory of Petroleum Resources and Prospecting, China University of Petroleum, Beijing*

Corresponding Authors: 1836857914@qq.com, rukuan_edu@163.com, xue_liang1983@163.com

In smart water-flooding, smart water-crude oil contact generates oil-in-water emulsion, which could effectively improve the displacement efficiency and sweep efficiency, and finally enhance oil recovery (EOR). Potential determining ions (PDIs) in smart water have a great influence on the stability of oil-in-water emulsion, however, their influence mechanisms have not yet reached a unified conclusion. To promote the optimization and application of smart water-flooding, the influence mechanisms of PDIs on the oil-in-water emulsion are studied. Fluorescence microscope observation, Water separation rate, Total organic carbon (TOC), Nanoparticle size measurement and ζ-potential measurement are combined to study the evolution process of oil-in-water emulsion in various brines (MgCl2, CaCl2, NaCl and Na2SO4 are dissolved into the deionized water, respectively, and the salinity is 500ppm-1000ppm-2000ppm-3000ppm-4000ppm-5000ppm-10000ppm-20000ppm-30000ppm). Through these experiments, the effect of PDIs on the oil-in-water emulsion stability can be obtained. More microscopic, Sum frequency vibration spectrum (SFG) is used to analyze the hydrogen-bonding network of the monolayer oil-water interface under the influence of PDIs. By this, the interaction mechanisms of crude oil-ion-water can be obtained in molecular scale. Experiment results showed that the PDIs in smart water-flooding have a great influence on the stability of oil-in-water emulsion. Thereinto, Mg2+ and Ca2+ promote the emulsion coalescence, and their promotion effect first strengthened and then weakened with the increasing concentration. There are optimal concentrations for Mg2+(3000ppm) and Ca2+ (2000ppm), corresponding to the fastest emulsion coalescence, the highest water separation rate, the least TOC content, the smallest stable emulsion size, the most suitable ζ-potential and the most obvious perturbation of ordering of the interfacial water molecules. Whereas, SO42- inhibits the emulsion coalescence and its inhibition effect strengthened with the increasing concentration. Meanwhile, it slightly enhances the ordering of the interfacial water molecules. Mg2+ and Ca2+, firstly, act as a bridge to promote the emulsion coalescence and their effect is most obvious at optimal concentration. Subsequently, the excessive Mg2+ and Ca2+ compress the electric double layer (EDL) and slow down the emulsion coalescence. SO42-, not only compresses the EDL, but also competes with polar crude oil components for Mg2+ and Ca2+, hence inhibits the emulsion coalescence. There is an optimal proportion of (Mg2+, Ca2+)/SO42-, which could shape the emulsion to a certain size and keep stable, meet the precise EOR requirements. From macroscopic to microscopic, this paper systematically explores the influence mechanisms of PDIs on the stability of oil-in-water emulsion in smart water flooding, which is of great significance not only for the optimization and application of the EOR technology, but also for many other industrial processes such as the treatment of the marine petroleum pollution and the optimization of the long-distance petroleum transportation.

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A (real) multi-scale solver for two-phase flow: a micro-continuum approach

Authors: Cyprien Soulaine[1]; Francisco Carrillo[2]; Ian Bourg[3]

[1] *CNRS - Earth Sciences Institute of Orleans*

[2] *Princeton Univeristy*

[3] *Princeton University*

Corresponding Authors: bourg@princeton.edu, cyprien.soulaine@gmail.com, franjcf@outlook.com

Micro-continuum approaches are intermediate between a pure Navier-Stokes description of flow and transport and a continuum-scale model using Darcy's law [1]. They use a unique formulation regardless of the content of grid cells, i.e. the same set of partial differential equations handles both pore-scale and Darcy-scale physics. Micro-continuum approaches are intrinsically two-scale allowing simulations with resolved and unresolved porosity in the same computational domain. For example, this hybrid-scale framework allows simulations in fractures (Stokes flow) surrounded by a porous matrix (Darcy's law) [1]. It is therefore well-suited to simulate flow and transport in micro-tomography images that contain sub-voxel porosity [2]. The technique can also move fluid / solid boundaries in presence of geochemical processes such as dissolution or precipitation [3,4]. Recently, solid mechanics have been introduced into the framework to model the hydrology of soft porous media such as clays and elastic membranes [5].

The micro-continuum frameworks so far were limited to single-phase flow only. In this work, we propose a multi-scale solver for two-phase flow in porous media based on a multi-phase micro-continuum model. The model is rooted in the elementary physical principles and rigorously derived using the method of the volume averaging. Eventually, we obtain a single set of partial differential equations that can be used both at the pore-scale and the continuum-scale and also in hybrid-scale modeling for which the porosity in some regions of the computational domain is fully resolved while some other regions are unresolved. Particular attention is paid to derive a comprehensive physics in the porous domain including unsaturated conditions, capillary, and gravity effects. The two-phase micro-continuum framework is verified through a series of test cases where reference solutions exist. We show that the multi-scale solver converges to the standard Darcy-scale solutions (Buckley-Leverett, capillary-gravity equilibrium, drainage in heterogeneous reservoir) when it is used in a coarse grid, and converges to the two-phase Navier-Stokes solutions (droplet in a flat surface, capillary rise, drainage with film deposition, two-phase flow in a complex porous structure) when it is used at the pore-scale.

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Impact of solvent extraction on the petrophysical analysis of lacustrine shale

Author: Hongguo Qiao[1]

Co-authors: Qinhong Hu [2]; Shengyu Yang [1]; binyu Ma [1]; wenzhong Han [3]; xiaohui Sun [1]; xiuchuan Zhu [1]; xiugang Pu [3]

[1] *Key Laboratory of Deep Oil and Gas, China University of Petroleum (East China)*

[2] *Deportment of Earth and Environmental Sciences, The University of Texas at Arlington*

[3] *PetroChina Dagang Oilfield Company*

Corresponding Author: 1789718487@qq.com

Compared with conventional petroleum reservoirs, shale is characterized by much lower porosity and permeability. Petrophysical analyses of shale is important in assessing the mobility and productivity of shale oil. However, the residual bitumen, including light hydrocarbons and heavy oil, often fills in the pores and fractures of the shale to influence the experimental determination of petrophysical characteristics.
As a Paleogene lacustrine shale deposited in the Bohai Bay Basin with a high organic matter content and considerable thickness, the Kongdian Formation holds a vast potential for shale oil in China. However, compared with productive shale oil plays in the United States, the Kongdian shale is featured by higher heterogeneity in facies, lower thermal maturity, and higher wax content. The knowledge about its petrophysical characteristics is essential in increasing the efficiency of shale oil exploration.
In this work, a series of experiments are designed to optimize the "oil-washing"method. Samples with different sizes from < 75 μm to 2.5 cm, are to be extracted with a commonly used solvent (93% dichloromethane:7% methanol in volume) to explore the penetration distance, and different extraction times to optimize the optimal extraction time. We will also conceptually compare the petrophysical characteristic of shale before and after extraction, using field emission-scanning electron microscopy (FE-SEM), mercury intrusion porosimetry (MIP), low pressure gas physisorption, and nuclear magnetic resonance (NMR). Changes in the porosity and permeability of shale in response of bitumen blocking and clay expansion are to be systematically revealed.

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Pore connectivity of shale oil reservoirs from small angle neutron scattering, mercury intrusion porosimetry and spontaneous imbibition experiments

Author: Xiaohui Sun[1]

Co-authors: QinHong Hu [2]; Binyu Ma [1]; Tao Zhang [3]; Mianmo Meng [3]; Shengyu Yang [3]; Xiugang Pu [4]; Wenzhong Han [4]

[1] *Key Laboratory of Deep Oil and Gas, China University of Petroleum (East China), Qingdao 266580, P.R. China*

[2] *University of Texas at Arlington, Arlington, TX 76019, USA*

[3] *Key Laboratory of Deep Oil and Gas, China University of Petroleum (East China), Qingdao 266580, P.R. China.*

[4] *PetroChina Dagang Oilfield Company, Tianjin 300280, P.R. China*

Corresponding Author: 1403964919@qq.com

Shale oil is mainly stored in micro-nano pores, and oil molecules migrate from matrix to the fractures through connected pores during the production. Connected organic pores could be water-wet, while inorganic pores water-wet. Thus, an understanding of the total pores, as well as connected organic and inorganic pores, are conducive to the understanding the shale oil production. Small angle neutron scattering (SANS) is used to obtain the total (both connected and "isolated") porosity, and mercury intrusion porosimetry (MIP) is the connected porosity, and spontaneous imbibition (SI) the pore connectivity of oil- and water-wet pore connectivity.
Working with Kongdian Formation lacustrine shale reservoir in Bohai Bay Basin in eastern China, the MIP experiments show that the porosity of shale is between 0.54% and 3.24%, with a predominant pore-throat size distribution from 2.8-50 nm. The estimated tortuosity increases rapidly with the increase of the critical pressure, and the geometric tortuosity is high, indicative of poor pore connectivity. Spontaneous imbibition experiments with different fluids (water-wet distilled water and oil-wet n-decane) indicate that the imbibition slopes, from the plot of log (imbibed mass) vs. log (imbibition time), with distilled water are around 0.25, while the imbibition slope of sandstone samples from conventional reservoir is about 0.5; therefore, the connectivity of water-wet pores is poor in Kongdian Formation. On the contrary, the imbibition slope of sample with n-decane is high, which ranges from 0.58 to 0.79 to indicate a good connectivity of oil-wet pores. The mixed behavior of much better oil than water wettability is confirmed from contact angle measurements. Our research contributes to the first appraisal of the fluid-wettable pore connectivity of lacustrine shale oil in China.

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Experimental Studies on Carbonated Smart Water-flooding Mechanisms in Tight Reservoir

Authors: Rukuan CHAI[1]; Yuetian LIU[2]; Liang XUE[2]; Jing XIN[3]

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

[2] *State key Laboratory of Petroleum Resources and Prospecting, China University of Petroleum, Beijing*

[3] *China Oilfield Services Limited*

Corresponding Authors: xinjingymp@163.com, 1836857914@qq.com, xue_liang1983@163.com, rukuan_edu@163.com

Tight reservoirs are widespread in China, but its recovery factor is always so low due to the poor physical properties. Hence, tight reservoir urgently needs an alternative, cheap and environmental friendly enhance oil recovery (EOR) technology. Carbonated smart water-flooding (CSW) is a new EOR technology that successfully combines smart water-flooding with carbonated water-flooding. This paper investigates the mechanism of carbonated smart water-flooding in tight reservoirs by experiments, from the macroscopic scale to the microscopic scale.
Firstly, macroscopic experiments, the long core displacement experiment, the interfacial tension measurement and the contact angle measurement are combined to study the influence of potential determining ions in carbonated smart water on the recovery factor, interfacial tension and contact angle. Then, microscopic experiments, the CO2 dissolution experiment in CO2-smart water system and CO2-crude oil-smart water system are respectively conducted to study the influence of the potential determining ions in smart water on the dissolution of CO2, as well as the partition coefficient of CO2 between smart water and crude oil.
Experiment results showed that the carbonated smart water-flooding can significantly improve the recovery factor of the tight reservoir, which is manifested by the synergy of carbonated water-flooding and smart water-flooding. Potential determining ions (Mg2+, Ca2+ and SO42-) in smart water present great importance in carbonated smart water-flooding performance. With the increase of Mg2+ or Ca2+, the recovery factor first increases and then decreases, the wettability improvement first strengths and then weakens, the interfacial tension first decreases and then increases, the CO2

dissolution in smart water and the partition coefficient of CO2 between crude oil and brine increases first and then decreases. The optimum Mg2+ and Ca2+ concentration are 2500ppm and 3500ppm. While, SO42- is double-edged, it promotes Mg2+and Ca2+ to improve wettability, but it results in the increase of interfacial tension and accompanied by the decrease of CO2 dissolution and partition coefficient of CO2 between crude oil and brine. There is an optimum of (Mg2+, Ca2+)/SO42-, which can maximize the effect of smart water-flooding by increasing the CO2 dissolution and the partition coefficient of CO2 between crude oil and brine, meanwhile optimize the carbonated water-flooding by enhancing the potential determining ions effect on wettability improvement and interfacial tension decrease.
This paper innovatively combines smart water-flooding with carbonated water-flooding into an alternative, cheap and environmental friendly EOR method, carbonated smart water-flooding. Moreover, the mechanism of carbonated smart water-flooding is systemically studied by experiments from the macroscopic scale to the microscopic scale. Due to its unique nature in EOR and CO2 sequestration, the hybrid technology has great research and application potential in the development of the tight reservoir.

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An experimental study of the interplay between viscous, capillary and gravitational forces in two-phase flow in a three-dimensional porous medium

Author: Joachim Falck Brodin[1]

Co-authors: Per Arne Rikvold [2]; Marcel Moura [1]; Knut Jorgen Maloy [1]

[1] *PoreLab*
[2] *Porelab*

Corresponding Authors: k.j.maloy@fys.uio.no, prikvold@fsu.edu, marcel.moura@fys.uio.no, j.f.brodin@fys.uio.no

We study the interplay between viscous, capillary and gravitational forces in two-phase flow in a three-dimensional porous medium, with the use of an optical scanner based on index-matched medium and fluorescent fluids. A more viscous, denser, fluid is injected into a less viscous, less dense fluid in a 3D porous medium, comprised of randomly packed glass beads of uniform size. We tune the injection rate over 10 experiments. Experience from the 2D scenario suggests that with a slow injection rate capillary and gravitational forces will dominate, and we should observe an unstable displacement and fingering. Conversely, with a high injection rate, viscous forces will dominate, leading to a more stable displacement and a narrower invasion front. How do the 2D findings hold up in the 3D scenario? We confirm the qualitative findings from the 2D experiments and establish a clear regime change, from unstable to stable displacement. We seek to derive a dimensionless number to quantify the relevant balance of forces and consider this number in relation to the invasion pattern. We characterize the invasion by Minkowski-functionals and fractal dimensions and seek relations between the found geometries and the derived dimensionless numbers.

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Micro-Scale Mechanism Analysis of NAPL Contamination Remediation in Heterogeneous Porous Media

Authors: Xiaopu Wang[None]; Xu Wang[None]; Yan Li[None]

Corresponding Authors: 17854229365@163.com, wxp@upc.edu.cn, wangxu314159@163.com

Oil spill accidents occur rather often in recent years, causing a large amount of toxic substances ((PAHs, PCBs , TPH) to enter the soil. These nonaqueous phase liquids (NAPLs) can attach to soil particles surface due to their high octanol / water partition coefficient and are difficult to eliminate from soil. Conventional physical and chemical treatments, influenced by soil heterogeneity, leave pollutants within less permeable regions in the subsurface. Thus, there is an urgent need to find an economic and efficient approach for NAPL-contaminated soil remediation.
Remediation with surfactant and chemotactic bacteria can improve the bioavailability of the NAPL pollutants in soil, providing a theoretically effective approach to solve the problem above. Surfactants can enhance the elimination of NAPL in the high and some of the low permeable regions, and chemotactic bacteria can accumulate around NAPL sources in low permeable regions by sensing the pollutant concentration gradient. We designed a series of 2D microfluidic devices with dual-permeability to simulate the heterogeneous soil contaminated with NAPL, and studied the efficiency of typical surfactants and chemotaxis bacteria to clear the NAPL contamination under different groundwater flow rates (Darcy flow).
Our experimental results showed that though distilled water could displace part of the oil in the high permeable region of the microfluidic device, no explicit decrease of oil in the less permeable region was observed under different water flow rates. Better displacement effects were obtained from surfactant usage, compared with pure distilled water flooding. We found that surfactant flooding could produce fingering phenomenon in the low permeable area, and the fingering extent was related to water velocity and surfactant concentration. We injected chemotactic bacteria suspension into the chip after the distilled water and the surfactant displacement, and found that considerable bacteria tend to accumulate at the interface between the high and low permeable regions after the water flooding; and more chemotactic bacteria was found in the low permeable region after the surfactant flooding, while no enrichment phenomenon was obtained from the nonchemotactic bacteria. Ultimately, coupling numerical simulation of multi-physics filed provided theoretical support for the experimental research. The simulation results were consistent with the experiments results, and presented similar bacterial breakthrough curve. Our findings help elucidate the role of chemotactic bacteria-surfactant remediation in accelerating oil-polluted soil treatment, providing a novel idea to improve the remediation of petroleum contamination, demonstrating that bioremediation using chemotactic bacteria is a potentially economical and effective strategy to remove petroleum pollutants from heterogeneous soil structure.

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Model reduction for nonlinear multiscale parabolic problems using dynamic mode decomposition

Authors: Mengnan Li[1]; Lijian Jiang[2]

[1] *Hunan university*

[2] *Tongji university*

Corresponding Authors: ljjiang@tongji.edu.cn, mengnanli@hnu.edu.cn

In this talk, a model reduction technique is presented to solve nonlinear multiscale parabolic problems using dynamic mode decomposition. The multiple scales and nonlinearity will lead to great challenges for simulating the problems. To overcome this difficulty, we develop a model reduction method for the nonlinear multiscale dynamic problems by integrating constraint energy minimizing generalized multiscale finite element method (CEM-GMsFEM) with dynamic mode decomposition (DMD). Using CEM-GMsFEM to directly solve multiscale nonlinear parabolic models involves dynamically computing the residual and the Jacobian on a fine grid. This may be very computationally expensive because the evaluation of the nonlinear term is implemented in a high dimensional fine scale space. As a data-driven method, DMD can use observation data and give an explicit expression to accurately describe the underlying nonlinear dynamic system. To efficiently compute the multiscale nonlinear parabolic problems, we propose a CEM-DMD model reduction by combing CEM-GMsFEM and DMD. The CEM-DMD reduced model is a coarsen linear model, which avoids the nonlinear solver in the fine space. It is crucial to judiciously choose observation in DMD. Only proper observation can render an accurate DMD model. In the context of CEM-DMD, we introduce two different observations: fine scale observation and coarse scale observation. In the construction of DMD model, the coarse scale observation requires much less computation than the fine scale observation. The CEM-DMD model using the coarse scale observation gives a complete coarse model for the nonlinear multiscale dynamic systems and significantly improves the computation efficiency.

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Characterisation of strongly disordered mesoporous solids with the serially-connected pore model (SCPM)

Authors: Henry R. N. B. Enninful[1]; Daniel Schneider [1]; Antonia Hoppe[1]; Dirk Enke[1]; Rustem Valiullin[1]

[1] *Universität Leipzig*

Corresponding Authors: dirk.enke@uni-leipzig.de, valiullin@uni-leipzig.de, henry.enninful@physik.uni-leipzig.de, che12clv@studserv.uni-leipzig.de, schneider.work@outlook.com

Phase transitions of fluids in mesoporous solids offer analytical tools for characterisation of pore space architecture in porous solids. Confinement effects render alterations to bulk fluid properties and serve as markers for understanding structure of porous constructs. While huge success has been achieved for ordered porous materials with the general adsorption isotherm (GAI), same cannot be said for disordered porous materials. Complexity in geometrically-disordered pore systems yields complex phase transition pathways via cooperativity effects and render the need for improvements beyond the GAI.

In this work, we study gas sorption (adsorption/desorption) and NMR cryoporometry (melting/ freezing) of water in a synthesised small-pore disordered mesoporous glass of mean pore size 4nm to validate the model for strongly disordered porous materials. We show that, regardless of the model as a statistically linear chains of pores, the SCPM efficiently and self-consistently reproduces all thermodynamic phase states on boundary transitions and scans. By this, we prove that the existence of very small necks in geometrically-disordered pores which cause the metastable nucleation of new phases are sufficient to effectively eliminate percolation effects.

Additionally, we show NMR cryoporometry measurements of water in a classical vycor porous glass and reveal the impact of percolation on the freezing phase transition. At the same time, we argue that the melting transition is negligibly affected by percolation phenomena due to efficient nucleation. This provides us with a means to identify the network effects and to establish the pore interconnectivity.

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A serially-connected pore model (SCPM) for characterising disordered mesoporous materials

Authors: Henry Enninful[1]; Daniel Schneider [1]; Richard Kohns [2]; Dirk Enke[1]; Rustem Valiullin[1]

[1] *Universität Leipzig*

[2] *Universität Leipzig, Philipps-Universität Marburg*

Corresponding Authors: schneider.work@outlook.com, dirk.enke@uni-leipzig.de, valiullin@uni-leipzig.de, richard.kohns@uni-leipzig.de, henry.enninful@physik.uni-leipzig.de

Characterisation of porous solids is an important step towards the optimization of mesoporous solids for applications in catalysis, molecular separations, adsorption, enhanced oil recovery, gas capture and storage and many more. For disordered porous solids, particularly, the current characterisation tools such as gas sorption employ the general adsorption isotherm (GAI) developed for ordered pore architecture. Complexity in pore structure, including its attendant cooperativity effects in thermodynamic phase transitions, results in a more complex characterisation paradigm than what the GAI presents.
Herein, we present the basics of the recently developed serially connected pore model (SCPM), which extends the GAI by incorporating cooperativity effects in phase transitions arising from pore complexity. As a model of statistically disordered linear chain of pores, the SCPM will be validated with experimental data from phase transitions in synthesized porous silica materials of similar pore construct, MCM-41. Analogous to gas sorption (adsorption/desorption) studies, solid-liquid phase transitions (freezing/melting) of water in porous materials will be utilised to correlate with the theoretical model. Particularly, a refined NMR cryoporometry approach to solid-liquid phase transitions studies is suggested. Additionally, we discuss the range of application of the SCPM to real disordered porous materials.

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A systematic investigation of the intrinsic flow properties of fractures using a combined 3D printing and micro-computed tomography approach

Author: Tomos Phillips[1]

Co-authors: Tom Bultreys [2]; Arjen Mascini [3]; Nathaniel Forbes Inskip [1]; Sabine den Hartog [1]; Niko Kampman [4]; Kevin Bisdom [4]; Veerle Cnudde [2]; Andreas Busch [1]

[1] *Heriot-Watt University*

[2] *Ghent University*

[3] *University of Gent*

[4] *Shell Global Solutions International B. V.*

Corresponding Authors: a.busch@hw.ac.uk, arjen.mascini@ugent.be, niko.kampman@shell.com, veerle.cnudde@ugent.be, s.den_hartog@hw.ac.uk, tp45@hw.ac.uk, kevin.bisdom@shell.com, n.forbes_inskip@hw.ac.uk, tom.bultreys@ugent.be

Geological storage operations spanning energy, nuclear material and carbon dioxide (CO2) storage, require meticulous understanding of the integrity of geological seals over a range of temporal and spatial scales. Fluid-conductive fault and fracture systems in otherwise low-permeability rocks may threaten seal performance and compromise subsurface storage projects. The understanding of these systems is complicated by the occurrence of anisotropic aperture distribution caused by inherent surface roughness. Difficulties predicting fluid flow through fractures stems from our limited understanding of the fundamental controls on their intrinsic permeabilities, and the prevalence, severity and complexity of hydromechanical responses arising from the coupling of multiphase flow, pore pressure and effective stress. In this study, we systematically investigated the effect of surface roughness on the transport properties of 3D-printed (Acrylonitrile Butadiene Styrene resin) fracture surfaces with micrometre surface roughness distributions. We printed 11 separate fractures, 7 of which are synthetically generated self-affine surfaces encompassing a range of fractal dimensions (Df = 1.2 to 2.4) observed in nature. The remaining 4 are acquired from micrometre-scale surface scans from natural fractures within the Carmel mudrock, a caprock from a natural CO2 leakage site in Utah, USA. Fluid flow experiments using single (brine) and multiple fluids (decane and brine) are undertaken to investigate the fluid pathways and interactions between each phase across a range of effective stresses (5 to 25 bar). We investigate the interplay between multiphase flow dynamics, surface roughness and hydraulic aperture distribution to gain insight into the intrinsic transport properties of fractures with different origins of roughness. Experiments are performed and imaged using a micro-computed tomography scanner (EMCT; (Bultreys et al., 2016)), where the results can be used to further the understanding of the governing parameters influencing fracture transmissivity, while also constraining surface roughness inputs for single- and multiphase fracture flow models.

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Pore-scale imaging of multiphase flow in porous media: wettability, minimal surfaces, displacement efficiency

Author: Qingyang Lin[1]

Co-authors: Branko Bijeljic [2]; Sam Krevor ; Steffen Berg [3]; Martin Blunt [1]

[1] *Imperial College London*

[2] *Imperial College*

[3] *Shell Global Solutions International B.V.*

Corresponding Authors: steffen.berg@shell.com, q.lin11@imperial.ac.uk, m.blunt@imperial.ac.uk, s.krevor@imperial.ac.uk, b.bijeljic@imperial.ac.uk

Recent developments in pore-scale imaging enabled more advanced characterization of multiphase flow in porous media. We injected oil and brine simultaneously into two Bentheimer sandstones (with/without wettability alteration) and Estaillades carbonate (with wettability alteration) to demonstrate that the high-resolution three-dimensional X-ray visualization techniques allows the pore structure, fluid distribution and capillary pressure to be captured and quantified. The observed pore-scale insights were combined with steady-state measurements of relative permeability to provide a complete characterization workflow. We demonstrate how the system wettability and local capillary pressure, which can be measured through measuring both contact angles as well as interfacial curvatures, can impact the fluid distribution and displacement efficiency.

For the Bentheimer sandstones with different wettability conditions, we compare the measured relative permeability, capillary pressure to demonstrate that the mixed-wet sample has a distinct geometric and thermodynamic contact angles, approximately, around 90⊠ and a low residual oil saturation value implying high displacement efficiency. We also observed the minimal surface phenomenon in the mixed-wet system where the oil/water interfaces are saddle-shaped with two opposite, but almost equal, curvatures in orthogonal directions. The mean curvature, which determines the capillary pressure, is low, but the shape of the interfaces ensures, topologically, well-connected phases, which helps to understand the favourable displacement. We then apply the similar analysis workflow for the Estaillades carbonate with altered wettability, which also contains sub-resolution porosity. The main challenges include complex pore geometry with much smaller pore sizes, and the impact of displacement due to pores below image resolution.

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Scaling Analysis of Immiscible Two-Phase Flow in Porous Media with Fractal Permeability Fields

Authors: Saman Aryana[1]; Yuhang Wang[1]; Jesse McKinzie[1]; Frederico Furtado[1]

[1] *University of Wyoming*

Corresponding Authors: furtado@uwyo.edu, jmckinzi@uwyo.edu, ywang23@uwyo.edu, saryana@uwyo.edu

Fluid mixing in porous media appears in many practical applications such as CO2 utilization and storage in subsurface formations. The mixing process is a consequence of velocity fluctuations owing to geological heterogeneities and mobility contrasts of the fluids. Heterogeneity of the permeability fields in natural rocks is often observed to be correlated in space with spatial distributions that may exhibit fractal behavior at the field scale. In this work, fractal permeability fields are generated using

the fractional Brownian motion model where the degree of heterogeneity is controlled by the Hurst exponent. Scaling relations are derived for the immiscible two-phase flow scenario based on the self-similarity of the permeability field. Monte Carlo simulations using high resolution numerical solutions to the classical multiphase formulation are used to validate these scaling relations. In the simulator, flow equation are cast in a vorticity-stream-function form where Fourier transform is used to solve the vorticity-stream-function equation. The advective flux in the transport equation is computed using a central-upwind scheme, where the intermediate values are constructed using a fifth-order weighted essentially nonoscillatory scheme. For each simulation case, scaled mean saturation profiles from numerical simulations appear to collapse onto a single curve, which supports the developed scaling relation.

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Pore-scale Simulation of Gas Flow in Microscopic Porous Media with Complex Geometries

Authors: Yuhang Wang[1]; Saman Aryana[1]

[1] *University of Wyoming*

Corresponding Authors: saryana@uwyo.edu, ywang23@uwyo.edu

Lattice Boltzmann method (LBM) is an efficient tool to perform direct numerical simulation of gas flow in micro-size pores. Despite great advances in LBM and its use in describing slip flow of gas in micro-size channels, few studies exist currently that provide formulations that are able to capture gas flow behavior in domains with complex boundary geometries. As a result, the Impact of complexities in pore structures on gas flow are not fully understood. In this study, we propose a modified second-order slip boundary condition with a new set of slip coefficients guided by solutions of the linearized Boltzmann equation. The proposed formulation is further validated against results from the direct simulation Monte Carlo method. In this work, we investigate gas flow behavior in the presence of with complex geometries by introducing obstacles of different shapes in the simulation domain. Velocity profiles at different locations in such a domain are in close agreement with results from molecular dynamics simulation reported in literature. The proposed LBM formulation is then used to investigate the slip velocity model in micro-size channels. To that end, a series of simulation runs is performed in both slip and transition flow regimes. Based on these numerical experiments, a new set of slip coefficients are reported for the slip model. Finally, this work is extended to the study of gas flow in porous media with complex geometries. Three types of boundary treatments, including the proposed second-order boundary scheme, as well as two widely used methods, i.e., the bounce-back and the Maxwellian diffusive reflection scheme, are implemented and compared. Results indicate that gas flow is strongly affected by the treatment of boundary conditions in the transition flow regime.

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Optimal Dispatch Techniques for Natural Gas Industry - Reservoir Simulation and Data Simulation

Authors: Tao Zhang[1]; Yiteng Li[1]; Shuyu Sun[2]; Hua Bai[3]

[1] *King Abdullah University of Science and Technology*

[2] *King Abdullah University of Science and Technology (KAUST)*

[3] *Beijing Oil & Gas Pipeline Control Center, China National Petroleum Company*

Corresponding Authors: tao.zhang.1@kaust.edu.sa, yiteng.li@kaust.edu.sa, shuyu.sun@kaust.edu.sa

The whole world is stepping into the Era of Industry 4.0, while new techniques including Big Data, Internet of Things and Artificial Intelligence are changing every aspect of our daily life. In order to meet the new challenges brought by this trend and overcome the air pollution problems always criticized by the public, the energy industry is now looking for clean resources. Natural gas, including shale gas, has attracted increasing attentions as a relative clean energy. Due to the special requirements in the storage and transportation of natural gas, dispatch systems should be controlled carefully to ensure the reliability at the same time of improving efficiency. A great strategy is now implemented throughout China's petroleum industry, to establish a modern dispatch system facilitated with big data techniques and intelligent control schemes. The whole industry chain of natural gas is involved in this wave of reform, from production, gathering, processing to transportation, storage and marketing. In this talk, we will investigate related approaches to show the potential research directions following this trend, and try to utilize the most advantages of modern big data techniques. Uncertainty quantification (UQ) is an important task in the designing of dispatch systems for natural gas industry, where many parameters are unknown or highly uncertain and a large number of factors are included in various processes of the chain correlated with multiple disciplines. Classical uncertainty quantification is no more applicable as the large number of realizations to be evaluated and the many cells for accurate description of flow and transport behaviors cannot be treated efficiently for a national scale platform and industry scale system. Our focus is now on alternative approaches, which are popularized worldwide in the Era of Industry 4.0 and capable of accelerating the optimal efficiency and reaction speed greatly using modern computational methods and facilities. We will try to decompose the whole technique scheme into different interrelated components, including reservoir simulation, data simulation, pipeline flow simulation and marketing simulation. Our goal is to suggest an optimal solution in each part and to figure out a better method to link up these components associatively.

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Dynamics of liquid bridge on moving porous substrates

Authors: Si Suo[None]; Yixiang Gan[None]

Corresponding Author: xjtu_ss@163.com

Liquid bridges are encountered in many industrial applications and natural processes, such capillary gripping, printing ink transfer and insects adhering or walking on the water surfaces. In this work, we focus on dynamics of the liquid bridge between a solid plane and a porous substrate, which is a complex process composed of liquid spreading, imbibition, drainage, and rupture. The phase field model is utilized to capture the dynamics of the liquid-gas interface, and this numerical framework is validated against the experimental observation. To exactly mimic the behavior of liquid transfer inside the porous region, a pore-scale model is built to represent the homogeneous porous substrate. Based on the simulation results, it is suggested that besides the surface wettability and substrate shape, the characteristics of porous media, i.e., permeability and capillary pressure, also control the dynamics of liquid bridges, especially the post-rupture water retention. To characterize the rupture patterns of a liquid bridge, we propose a non-dimension number that combining the above factors and pinpoint the water retention ratio quantitively. The present study provides an alternative practical way to control the water retention for various applications, e.g., increasing efficiency of water collection, or improving stain removal.

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Experimental studies on gas dissipation during the coring process of shale

Author: Ying Sun[1]

Co-authors: Renyuan SUN [2]; Shuxia Li [1]; haoyang ma [3]; Xiaobing Wang

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

[2] *School of Petroleum Engineering*

[3] *CHINA UNIVERSITY OF PETROLEUM*

Corresponding Authors: s19020113@s.upc.edu.cn, sunying009@outlook.com, 407709436@qq.com, sunrenyuan@126.com, 13864886881@163.com

The shale gas content is an important indicator of shale gas exploration and reservoir evaluation, directly affecting gas well productivity, production calculation and gas well life. So, accurate calculation of shale gas content is very important to determine the production methods of shale gas reservoirs. In this study, the self-designed CSG shale gas content simulation experiment system was used to simulate the process of the coring from different depths at different rates to desorption tank. Shale samples from Cen Gong block, Guizhou, were selected to analyze the influence of formation pressures (4 MPa and 6 MPa) and pressure drop rates (0.5 MPa/min, 0.4MPa/min, 0.3MPa/min, 0.2MPa/min, 0.1MPa/min and 0.05MPa/min) on the amount of shale gas lost during this process. Through the depressurization mining experiment, the desorbed gas volume and residual gas volume of shale were obtained, and then the influence of formation pressure, core rate and escape time on the calculation of shale gas content was obtained. The changes of the proportion of lost gas, desorbed gas and residual gas under different conditions was analyzed. The results show that under the same pressure, with the increase of pressure drop rate, the proportion of lost gas declines, while the proportion of desorbed gas increases. The proportion of residual gas increases with the decrease of the escape time under low pressure conditions, and it decreases with the decrease of the escape time under high pressure conditions. There is a turning point in the proportion of loss gas and desorbed gas. Before the turning point, the proportion of loss gas and desorbed gas changes rapidly with the pressure drop rate increases. After the turning point, the variation range tends to be gentle. And the pressure increases, the pressure drop rate corresponding to the turning point increases. There is a stable production stage in the gas production process, which is represented by a gas production rate step, and the shorter the escape time, the higher the gas production rate corresponding to the stable production stage, and the shorter the stable production time, the faster the gas production ends. This study has great significance for the objective evaluation of shale gas content and the proportion of different gases, and can provide a theoretical basis for reserves evaluation and production decline analysis.

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Hydraulic behaviour of sand-biochar mixtures: Particle size effects on permeability

Authors: Ziheng Wang[1]; Majid Sedighi[1]; Amanda Lea-Langton[1]

[1] *The University of Manchester*

Corresponding Authors: amanda.lea-langton@manchester.ac.uk, majid.sedighi@manchester.ac.uk, ziheng.wang@manchester.ac.uk

Understanding the hydraulic behaviour of soils amended by biochar is important in agriculture sector where biochar is introduced to the soil balance the water retention and hydraulic properties. Other potential applications such as the use of sand-biochar in water filtration systems would require an accurate description of flow characteristics. Biochar normally contains a large volume of pores which are smaller than 30 μm that contribute limitedly to the overall water flow. The pore characteristics of biochar have considerable effects on the permeability of soil-biochar mixtures.
The results of a series of experimental investigation will be presented which aim to improve the understanding of particle size effects on permeability of sand-biochar mixtures. The experiments presented include a series of constant head permeability tests on a range of sand-hardwood biochar mixtures with different grain size distributions. The particle size distributions range between 0.063 mm and 8 mm with coefficient of uniformity of 3.3.We will demonstrate that there are two critical ranges of biochar volumetric contents at which the permeability of mixture would either increase or decrease by increasing the biochar content. The permeability of biochar-sand mixture can fall to 15% of that of original pure sand even if the particle size of biochar was considerably larger than that of sand.
The conventional models sued to describe the permeability of biochar-amended soils are largely based on correlations with total porosity. Our results show that the applications of such correlations yield unsatisfactory predictions. We will propose correlations between key particle size characteristics including D10 (diameter of particle size at 10% passing) and D60 (diameter of particle size at 60% passing) of the sand biochar mixtures and permeability.

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Study of the effect of pore-scale mineral wettability alterations on the relative permeability curves

Authors: Ming Fan[1]; James McClure[1]; Ryan Armstrong[2]; Mehdi Shabaninejad[3]; Li Zhe[1]; Laura Dalton[4]; Dustin Crandall[4]; Cheng Chen[1]

[1] *Virginia Tech*

[2] *University of New South Wales*

[3] *Australian National University*

[4] *National Energy Technology Laboratory*

Corresponding Authors: laura.dalton@netl.doe.gov, dustin.crandall@netl.doe.gov, mcclurej@vt.edu, chen08@vt.edu, mehdi.shabaninejad@anu.edu.au, mingfan@vt.edu, rexl@vt.edu, ryan.armstrong@unsw.edu.au

Injection of carbon dioxide (CO2) into geological formations has been recognized as one of the most practical approaches to reduce greenhouse gas emissions and mitigate resultant climate change. During CO2 sequestration process, it has been acknowledged that mineral surfaces can undergo wettability alteration. Thus, the wettability of CO2 can vary considerably from complete water-wet to almost CO2 wet, which gives rise to large uncertainty in storage capacity and sealing integrity. Therefore, it is of key importance to understand the wettability of mineral surfaces in subsurface multiphase flow and transport.

Mt.Simon sandstone is a favorable storage reservoir for CO2 sequestration in the midwest of USA, because of its advantages in depth, thickness, permeability, and bounded impermeable caprocks. In this study, a Mt.Simon sandstone was first scanned with X-ray micro-computed tomography (micro-CT) scanning and then the sample mineralogy distribution, composition, and texture were classified with Quantitative Evaluation of Minerals by Scanning Electron Microscopy (QEMSCAN). Through QEMSCAN analysis, it is observed that Mt.Simon mainly comprises clay (10.7%), quartz (67.3%), feldspar (13.8%), micas (3.4%), and mixing group including pyrite and other high density minerals. The clay minerals are composed of randomly distributed amorphous particles and have a large surface area to volume ratio and high surface roughness, which has a large influence on relative permeabilities for both wetting and non-wetting fluids during wettability alterations.
In this study, the 3D pore structure information was extracted from micro-CT images and then used as interior boundary conditions of flow modeling in a pore-scale LB simulator to simulate multiphase flow within the pore space. The wettability of clay, quartz, and feldspar surfaces are modified with strongly water-wet, intermediate-wet, and oil-wet conditions. Due to the complex clay geometry, the changes in relative permeabilities are observed. When the contact angle of clay minerals increased, both the wetting and non-wetting fluid relative permeability curves moved to the left. The wettability alteration for other major minerals quartz and feldspar are also examined. Then, the continuous connected and trapped nonpercolating subphases for the wetting and non-wetting fluid relative permeabilities are analyzed. The combination of micro-CT imaging and LB multiphase flow simulations is a promising tool for advancing fundamental understanding of the mineral wettability alterations that regulate multiphase flow in complicated reservoir rocks.

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Study on tight oil seepage characteristics based on digital cores

Authors: Yixin Cao[None]; Ning Qi[None]; Xinlei Yuan[None]

Corresponding Authors: 452597144@qq.com, 1643112048@qq.com, 1430067486@qq.com

Micron CT was selected to scan the sample, and after obtaining the CT scan image, the digital core can be established. The modeling and preparation process can be divided into image processing, characterization unit analysis, digital core establishment of pore structure and ball-and-stick model establishment.
The pore threshold was optimized based on SEM image, mineral threshold was optimized based on EDX image, and pore threshold was optimized based on nuclear magnetism and mercury injection experimental data. Finally, a synthetic core is constructed according to the optimized data.
LBM is a mesoscopic model between the microscopic molecular dynamics of fluids and the macroscopic continuum method, which is very suitable for simulating the behavior of multiphase fluids in complex systems. On the basis of the 3d digital core, the simulation of seepage flow based on the LBM model is carried out, and the correlation and continuity of the conclusions are guaranteed.
The convolutional neural network (CNN) based on the deep learning theory is the first deep learning algorithm that has truly successfully trained the multi-layer network structure. When connecting

the CT scan images of core samples with the seepage characteristics, the CNN algorithm is an appropriate link. The training parameters of CNN are reduced, the generalization ability of the model is stronger, the pooling operation reduces the spatial dimension of the network, and the translation invariability of the input data is not required. Is the most suitable deep learning method applied to the evaluation of seepage characteristics in tight reservoirs, and the input end is the CT scan data of samples. The key to solving core CT image recognition with image deep learning is to transform the problem of microscopic pore throat structure recognition and simulated seepage characteristics into the problem of target detection in the field of image recognition.

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On volume averaging modelling of porous electrodes –intrinsic phase average and macroscopic flux definition at solid/electrolyte interface

Authors: Xiaoguang Yin[None]; Zeyong Wang[1]; Thomas Sweijen[2]; S. Majid Hassanizadeh[2]; Baohua Li[3]

[1] *Convergent Science*

[2] *Utrecht University*

[3] *Tsinghua Shenzhen International Graduate School*

Corresponding Authors: smhfba@yahoo.com, xiaoguang.yin@sz.tsinghua.edu.cn, t.sweijen@uu.nl, libh@sz.tsinghua.edu.cn, zeyong4c@gmail.com

Macrohomogeneous description of porous electrodes can be derived by volume averaging of pore-scale equations. Two aspects of volume averaging modelling of porous electrodes are examined. One aspect is intrinsic phase average. A porous electrode is considered as two overlapping continua: a solid electrode and an electrolyte. So, intrinsic phase average properties are assigned to the centroid of averaging volume and the centroid of that phase. The underlying assumption that these two centroids coincide with each other could be problematic for heterogeneous systems. This effect is illustrated by applying Darcy's law to describe single phase flow under gravity in heterogeneous porous structure. Another aspect is the macroscopic flux definition at solid matrix/electrolyte interface. Flux should be averaged over interface. However, macroscopic flux is usually defined based on volume-averaged quantities for convenience. Our results show that significant discrepancy could exist between these two flux, resulting in disagreement between microscale and macroscale. Clarification of these two aspects could provide a more solid foundation for porous electrode theory and aid in interpreting experimental and simulation data between pore scale and macrohomogeneous scale.

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Pore structure characteristics of the Paleogene Shahejie Shale Oil Formation in Dongying Sag, Bohai Bay Basin, China

Author: Xiuchuan Zhu[1]

Co-authors: Qinhong Hu [2]; Mianmo Meng [3]; Na Yin [4]; Binyu Ma [3]; Yushan Du [5]; Jing Chao [5]

[1] *17862106280*

[2] *The University of Texas at Arlington,*

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

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

[5] *Shengli Oilfield, SINOPEC*

Corresponding Author: xiuchuan9702@163.com

Abstract: The pore structure characteristics of lacustrine oil shales in eastern China are not studied in detail, and this work used integrated approaches of mercury intrusion porosimetry (MIP) and nuclear magnetic resonance (NMR) to achieve the research objectives. More than 20 core samples were selected from Paleogene Shahejie Formation in Dongying Sag of Bohai Bay Basin, which is under investigations for shale oil exploration. The porosity, pore size distribution, permeability, tortuosity, and movable fluid saturation were analyzed. MIP results show that samples have two pore types of nano and macro-pores. Related to shale matrix, the nanopores range from 6 to 20 nm in their pore-throat sizes, and is comprised of 76.3% of the total pore volume. The macropores are distributed at 10-50 μm in pore-throat sizes, probably related to the microfractures or lamination. The low efficiency of mercury withdrawal ranges from 6.97% to 27.5%, and the average tortuosity of samples is 7.86, indicating complicated pore structure NMR T2 spectra of samples have two or three peaks, and the latter are the dominant one. The first two peaks are mainly between 5 nm to 30 nm, and the third peaks are about 9 μm. The movable fluid saturation, porosity and permeability of laminated shale samples are 76.4%, 5.45%, and 0.695 mD, as compared to 53.8%, 4.89%, and 0.0249 mD for the blocky shale samples. The lamination has a strong influence on permeability and less impact on porosity. Based on above researches, shale reservoirs with lamination will be beneficial to oil production in the study area.

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An analytical fractal model for water transport in shale reservoirs

Author: Fanhui Zeng[1]

Co-authors: Yu Zhang [1]; Jianchun Guo [1]; Yu Zhang [1]; Wenxi Ren [1]; Jianhua Xiang [2]

[1] *State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu, China*

[2] *Engineering Technology Research Institute, Chengdu, China*

Corresponding Authors: guojianchun@163.com, xiangjh@petrochina.com.cn, zq1819096@163.com, zengfanhui023024@126.com, zhangyu0971@126.com

We investigate the ALP (apparent liquid permeability) for shale porous media composed of inorganic and organic materials in this paper. The ALP model is developed to reveal water transport mechanisms in shale porous media on the basis of water behavior transport through a single nanotube. The present model takes into account effective slip length effect related to Nano pore size and wettability, total organic carbon content (TOC), structural parameters and also confined fluid viscosity varied with pore size. The proposed model is successfully validated against the published simulation data. The exhibits that: (1) The confined fluid transport capacity increase with contact angle and maximum pore size decrease, and the value can be several times larger than that of bulk water for organic matter. (2) The ALP enhanced with TOC content for the effective slip length and varying viscosity have positive effect on shale organic matter permeability. (3) The fluid transport capacity is strongly dependent on pore structure size, such as capillary size, porosity, fractal dimensions of pores. The value is increase with pore/capillary size, porosity, while decrease with pores fractal dimensions.

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A unified multiple transport mechanism model for gas through shale pores

Author: Fanhui Zeng[1]

Co-authors: Yu Zhang [1]; Jianchun Guo [1]; Qiang Zhang [1]; Wenxi Ren [1]; Jianhua Xiang [2]

[1] *State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu, China*

[2] *Engineering Technology Research Institute, Chengdu, China*

Corresponding Authors: xiangjh@petrochina.com.cn, zq1819096@163.com, zengfanhui023024@126.com, guojianchun@163.com, zhangyu0971@126.com

Predicting apparent gas permeability (AGP) in nanopores is a major challenge for shale gas development. Considering the differences in the gas molecule-pore wall interactions in inorganic and organic nanopores, the gas transport mechanisms in shale remain unclear. In this paper, gas flow channels in shale, which are separated into inorganic pores and organic pores, are treated as nanotubes. Inorganic pores are assumed to be hydrophilic, and organic pores are assumed to be hydrophobic. In organic pores, multiple bulk free gas and surface adsorbed gas transport mechanisms are incorporated, while the bulk gas and water film are considered within inorganic pores. This paper presents a unified multiple transport mechanism model for both organic nanopores and inorganic nanopores; these models consider the absorption, stress dependence, real gas and water storage effects on gas transport comprehensively for the entire flow regime. The results are validated with published data which is more in line with the real situation.

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Visualizing 3D distribution of wet domain in microporous layer in polymer electrolyte fuel cell by X-ray computed tomography under water vapor supply

Author: Satoru Kato[1]

Co-authors: Satoshi Yamaguchi [1]; Wataru Yoshimune [1]; Yoriko Matsuoka [1]; Akihiko Kato [1]; Yasutaka Nagai [1]; Takahisa Suzuki [1]

[1] *TOYOTA Central R&D Labs., Inc.*

Corresponding Authors: e1238@mosk.tytlabs.co.jp, e1062@mosk.tytlabs.co.jp, e1666@mosk.tytlabs.co.jp, e1325@mosk.tytlabs.co.jp e1707@mosk.tytlabs.co.jp, e4553@mosk.tytlabs.co.jp, e0964@mosk.tytlabs.co.jp

The cell potential of polymer electrolyte fuel cells (PEFCs) decreases by accumulation of liquid water in the cathode gas diffusion layer (GDL), which is usually composed of a substrate and a microporous layer (MPL). Although it is well known that MPLs suppress water accumulation in the GDL, the mechanism has not yet been fully clarified. It is therefore desirable to visualize 3D water distribution in both MPLs and substrates in designing and developing GDLs. The 3D water distribution in the substrate was conventionally visualized by operando (during the measurement of the performance) or ex situ (after liquid water injection) X-ray computed tomography (CT). However, operando X-ray CT is difficult to visualize 3D water distribution in the MPL. This is because the CT image of the MPL near the catalyst layer (CL) is blurry due to the strong X-ray absorption by Pt loaded in the CL. Although this problem can be avoided by the ex-situ visualization of liquid water injected into the MPL, injecting water into the hydrophobic and small pores of the MPL is difficult because the water injection requires high pressure in water.
Here we report a new ex-situ method in order to visualize the 3D distribution of the wet domain in the MPL. The experiment was conducted under water vapor supply instead of injecting liquid water. Problems in the conventional methods mentioned above are circumvented because the new method does not need either of the CL or the water injection with high pressure. The visualization results revealed that the MPL wetted heterogeneously. This heterogeneous wettability has not been reported in previous literature, and has not been predicted by mathematical models either. The latter is due to that the conventional models assumed structural and chemical properties of the MPL as homogeneous. The results will guide the future model development. In addition, the liquid water distribution in the through-plane direction indicated that liquid water formed in the MPL drained to not only substrate side but also outer surface side. This phenomenon gives new insight into the water accumulation at the interface between the MPL and CL, which is recently considered as one of reason for decreases of cell potential. The new method in this work is expected to be informative to understand water accumulation in the MPL.

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Pore scale study of multiphase and multicomponent transport in methane hydrate bearing sediment

Author: Junyu Yang[1]

Co-authors: Lin Shi [1]; Zhiying Liu [1]; Qianghui Xu [1]; Cheng Zan [2]

[1] *Department of Energy and Power Engineering, Tsinghua University*

[2] *Research Institute of Tsinghua University in Shenzhen*

Corresponding Authors: rnxsl@mail.tsinghua.edu.cn, yang-jy17@mails.tsinghua.edu.cn

Understanding of methane hydrate dissociation process in sediment porous media is crucial for evaluation of hydrate reservoir stability and prediction of hydrate resources exploitation. In this work, a pore scale numerical model based on lattice Boltzmann method is developed to investigate multiple physicochemical processes during methane hydrate dissociation, including gas-liquid multiphase flow, mass transport of dissolved methane and heterogeneous dissociation reaction on hydrate surface. Different distributions of methane hydrate in the porous media including pore-filling and grain-coating models are used to analyze the effect of hydrate construction on the dissociation process while multiphase distributions, concentration field and pore structure evolution are presented. In addition, the effects of initial pressure and wettability are investigated. Finally, parameters for continuum models including efficient dissociation rate and absolute permeability at different hydrate saturation in the processes are calculated. The pore scale studies of methane hydrate dissolution help to understand the multiple physicochemical processes with diverse affecting factors and provide theoretical direction for continuum models.

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Experimental study on evolution law of key parameters and characterization of initial gas desorption of coal particles

Author: Chaojie Wang[1]

Co-authors: Xiaowei Li [2]; Changhang Xu [1]; Yue Niu [3]

[1] *China University of Petroleum*

[2] *China University of MIning and Technology*

[3] *China University of Mining and Technology*

Corresponding Authors: ttgnhm@126.com, name_niuyue@163.com, changhangxu@upc.edu.cn, superj_wang@163.com

Generally, a coal and gas outburst only lasts for a few or tens of seconds from initiation to termination. To obtain the law of gas desorption from coal masses in the instantaneous outburst process, the gas desorption test of tectonically-deformed and primary-undeformed coal masses in the first 13s was carried out by using self-assembled gas desorption equipment. The experimental results show that for both coal masses, in the gas desorption process as the gas pressure increases, the drop rate of gas pressure slows down and the minimum value and the final stable value of temperature of the coal masses become lower. Under the same gas pressure, for primary-undeformed coal masses the drop rate of gas pressure decreases faster and the minimum value and the final stable value of temperature are generally higher. In addition, with the increase of gas pressure, the gas desorption amount is larger and the gas velocity in desorption become faster. For the same gas pressure, the gas velocity of tectonically-deformed coal masses is greater than that of primary-undeformed coal

masses. Meanwhile, the mass flow rate at the beginning of gas desorption increases with the increase of gas pressure and the mass flow rate of tectonically-deformed coal masses is about 2 times of that of primary-undeformed coal masses. The relationship between the mass flow rate and gas pressure is in accordance with the power function formula; for tectonically-deformed coal masses, the influence of gas pressure on the mass flow rate is greater than that of primary-undeformed coal masses. The relationship between desorption mass flow amount and the time is in accordance with the exponential function formula. Finally, it can be obtained that in the initial gas desorption process of coal masses, the relationship between desorption accumulation amount and the time is closely consistent with Langmuir formula.

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The topological origin of anomalous transport: Persistence of β in the face of varying correlation length.

Author: yaniv edery[1]

[1] *Technion*

Corresponding Author: yanivedery@gmail.com

Traditional concepts for flow in porous media assume that the heterogenous distribution of hydraulic conductivity is the source for the contaminant temporal and spatial heavy tail, a process known as anomalous or non-Fickian transport; this anomalous transport behavior can be captured by the β parameter in the continues time random walk (CTRW) framework. In previous studies we showed that there is a functional form relating the β parameter to the permeability variance (1) and fracture alignment in fracture fields (2). Moreover, we showed that this variance is strongly influencing the reaction pattern during transport (3). This study shows that as the spatial correlation length, between these heterogeneous distributions of hydraulic conductivities, increases, the anomaly of the flow reduces, yet the β value is unchanged suggesting that there is a topological component to the flow field, captured by the β. This finding is verified by an analysis of the flow field, showing that the changes in the conductivity values have little effect on the flow field morphology, which points to the topological component in the flow.

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Effect of proppant wettability on fines transport and retention in propped fractures during gas–water two-phase flow in coalbed methane reservoirs

Authors: Fansheng Huang[1]; Changyin Dong[1]; Xiaosen Shang[1]

[1] *School of Petroleum Engineering, China University of Petroleum (East China)*

Corresponding Authors: shangsen@upc.edu.cn, dongcy@upc.edu.cn, fansheng.huang@upc.edu.cn

Hydraulic fracturing is an effective way to improve the productivity of coalbed methane (CBM). However, during gas–water two-phase flow, massive invasion and retention of coal fines in propped fractures can lead to a sharp reduction in fracture conductivity. Herein, a long-term and effective method was proposed to control fines retention by modifying the wettability of proppant. Standard quartz sand was used as proppant carrier, and its wettability was modified to superhydrophilicity and superhydrophobicity by coating it with nano-SiOx and fluorocarbon, respectively. Three sets of experiments on coal fines transport in untreated proppant pack, superhydrophilic proppant pack, and superhydrophobic proppant pack were systematically conducted. During each experiment, a suspension of coal fines in water was coinjected with gas, and fines breakthrough concentration was carefully monitored. Experimental results revealed that the largest and the lowest breakthrough concentrations of coal fines were observed for superhydrophobic proppant pack and superhydrophilic proppant pack, respectively, indicating a reduction of fines retention with increasing hydrophobicity of proppant. Different from that in single-phase water flow, a series of moving gas–water interfaces (GWIs) is observed in gas–water two-phase flow. These moving GWIs play a significant role in fines detachment. Forces/torques acting on coal fines during the passage of GWIs, including encouraging forces (i.e., surface tension force and hydrodynamic force) and resisting forces (i.e., extended-DLVO force and frictional force), were analyzed to elucidate the effect of proppant wettability on fines mobilization. Theoretical results revealed that the ratio between encouraging torque and resisting torque acting on coal fines increases with the hydrophobicity of proppant. In other words, moving GWIs can lead to easier mobilization of coal fines, eventually fewer fines remain in propped fracture when the hydrophobicity of proppant strengthens. Notably, experimental data were well supported by theoretical results. This study presents the significant potential of superhydrophobic proppant in alleviating clogging of propped fractures, while enhancing fines transport during CBM production.

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Nanopore Connectivity and Fluid Migration in Shales

Author: Qinhong Hu[1]

[1] *University of Texas at Arlington*

Corresponding Author: maxhu@uta.edu

Nearly 40 years of American experience in shale development indicates a steep initial production decline and low overall recovery of hydrocarbons, which can be implicated by the complexity of nanopore structure (geometry and connectivity) and "dalmatian"wettability of shale formations. Working with several fluids (gas, mercury, Wood's metal, polar water, non-polar n-decane and toluene, and bi-polar tetrahydrofuran) and approaches (fluid invasion for edge-accessible effective porosity, small-angle neutron scattering for total porosity), we've been systematically studying the characteristics, as well as the interplay, of pore connectivity and wettability of leading shales in the United States (Barnett, Bakken, Eagle Ford, Haynesville, Mancos, Marcellus, Niobrara, and Spraberry-Wolfcamp). The approaches include pycnometry (liquid and gas), pore and bulk volume measurement after vacuum saturation, porosimetry (mercury intrusion porosimetry, low-pressure gas ph-

ysisorption isotherm, nuclear magnetic resonance cyroporometry), imaging (field emission-scanning electron microscopy, Wood's metal impregnation), scattering (ultra- and small-angle neutron scattering), and the utility of both hydrophilic and hydrophobic fluids as well as fluid invasion tests (imbibition, diffusion, vacuum saturation) followed by laser ablation-inductively coupled plasma-mass spectrometry imaging of different nm-sized tracers. A shale can have a good pore connectivity for a wetting fluid, but poor connection for a non-wetting fluid. Furthermore, pore spaces of different wettability are very likely associated with the compositions of shale such as organic matter, carbonates and clays. In other words, oil-wet pores are smaller (~5 nm) and yet well-connected, while water-wet pores are larger (~20 nm) but sparsely-connected. As a function of sample size, the low pore connectivity of shale also creates an extensive presence of isolated pores, and this associated steep decline of edge-accessible connected pore space is implicated in steep initial production decline and low overall recovery of hydrocarbons in shales.

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Fracture-matrix interactions implicated by matrix pore connectivity: From waste repository to shale hydrocarbon production

Author: Qinhong Hu[1]

[1] *University of Texas at Arlington*

Corresponding Author: maxhu@uta.edu

In low-permeability unsaturated fractured rock, fluid flows predominantly through the interconnected fracture network, with some fluid imbibing into the neighboring matrix rock. Imbibition (driven by capillary pressure gradient) advectively transports chemicals from fracture into matrix. Diffusion (driven by concentration gradient) can diffusively transport chemicals into the matrix. Once in the matrix, sorbing chemicals can sorb onto matrix rock. All these interacting processes (imbibition, sorption, and diffusion) are important to understand in the naturally and hydraulically fractured low-permeability rock. Pore structure of rock matrix integrates both geometry and topology of the pore network of the matrix, giving rise to emergent first-order effects on fluid flow and chemical transport in the matrix. Low permeability media make it likely that flow and transport is limited by pore topology (e.g., density of connections) rather than geometry (e.g., radius). Microscopic characteristics of porous materials –pore shape, pore-size distribution, pore connectivity – influence macroscopic behavior of fluid flow and chemical transport, and therefore affect the performance of geological repository with natural fractures and exploration-production of hydrocarbons in hydraulically-fractured shales.
This work discusses various, and complementary, approaches to investigating matrix pore connectivity of Yucca Mountain welded tuff of Nevada as well as Barnett, Eagle Ford, and Wolfcamp Shales of Texas, and the resulting anomalous behavior in fracture-matrix interactions. The experimental approaches include mercury intrusion porosimetry and Wood's metal impregnation, as well as traced imbibition and tracer diffusion followed with micro-scale elemental mapping with laser ablation-ICP-MS. These porous media have a disparate range of porosity, permeability, and pore structure characteristics. Measured porosity, permeability and median pore-throat size are as follows: 10.0%, 8.31×10-19 m2, and 47 nm for welded tuff; and 5.97%, 4.96×10-21 m2, and 9.1 nm for Barnett Shale. But pore size is not the major contributor to slow fluid flow and chemical transport, the anomalous fluid imbibition and chemical diffusion appear to be caused by low pore connectivity in the Barnett Shale, as shown from steep decline of edge-accessible porosity from vacuum saturation, the presence of only trace amount of diffusing solutes beyond a few mm from a sample edge, and ~400 μm penetration of Wood's metal even under a pressure of 6,000 bars. In summary, low matrix pore connectivity and associated fractured flow-transport behavior will dictate how low-permeability media will perform in natural and engineered systems such as waste repository and shale development.

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Characterization of capillary flow within hybrid woven screens in vertical and horizontal directions

Author: Ye Wang[1]

Co-authors: Yilin Lin [1]; Guang Yang [1]; Jingyi Wu [1]

[1] *Institute of Refrigeration and Cryogenics, Shanghai Jiao Tong University*

Corresponding Authors: jywu@sjtu.edu.cn, 840718627@qq.com, y_g@sjtu.edu.cn, wangyeee@sjtu.edu.cn

The screen channel liquid acquisition device (LAD) is one of the most promising technologies that achieves full liquid propellant acquisition under micro-gravity. The wicking performance of the metal woven screen is of great significance to recover the dried-out screens due to evaporation, since only fully wetted screens can block the bubbles. In this study, horizontal liquid spreading experiment and vertical isothermal wicking experiment are carried out with HFE-7500 as test fluid by measuring the volumetric liquid intake into the structured surface with a high speed camera and by measuring the wicking mass with an electronic balance, respectively. Hybrid wicking structures are manufactured using copper woven screens by surface roughening through chemical etching and by surface energy reduction through chemical modification.

From the microscopic point of view, the surface topography and micro-structures of the manufactured woven screens are studied by scanning electron microscope (SEM). The wetting behavior are theoretically analyzed based on the morphology of the porous screens. Extending to a macroscopic perspective, the metal woven screen, a thin porous layer through which the liquid spreads, is described by three structural macroscopic parameters, namely porosity, capillary diameter and permeability. The volumetric flow rate and the wicking distance are quantitatively investigated to characterize the wicking performance. Moreover, the influence of the gravity and the difference between the radial and linear capillary flow behavior are also studied. Results indicate that, the maximum reachable height, with the effect of gravity, and the wicking velocity, in both radial and linear directions, are augmented due to the increased surface wettability by creating nano-grasses and micro-cavities on the screen surfaces. Specifically, the hydrophilicity of the structured surfaces affects the wicking performance by influencing the contact angle in the capillary model. Considering the variable wicking velocities in perpendicular and diagonal directions of the woven structures, the equivalent capillary diameter of the screens are obtained according to the radial capillary-driven flow experiment. The superior wicking performance of the manufactured porous screens, by increasing the hydrophilicity, may provide a new direction for LAD screen selection and optimization.

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A New Fractal Model for Pore Structure and Capillary Tortuosity in Porous Media

Authors: Peng Xu[1]; Shuxia Qiu[2]

Co-authors: Min Wang [1]; Boming Yu [3]; Yuqing Shen [1]

[1] *China Jiliang University*

[2] *University of Shanghai for Science and Technology*

[3] *Huazhong University of Science and Technology*

Corresponding Author: xupeng@cjlu.edu.cn

Fractal geometry has been successfully applied to characterize the structures and investigate the transport properties of porous media due to its scale invariant property. An generalized fractal model for pore structure and capillary tortuosity is developed, and the fractal dimensions for pore size distribution and tortuous capillaries are introduced. A new fractal scaling law between the cumulative pore volume ratio and pore size is proposed. The pore fractal dimensions are determined with the proposed fractal model based on experimental results of sludge porous samples by low-field nuclear magnetic resonance (NMR) technique. And the relationship between tortuosity fractal dimension and porosity as well as pore fractal dimension is derived according to the capillary bundle model and equivalent pore-throat model. The results indicate that the pore fractal dimension increases with porosity under fixed pore size range, it is larger than 2.6 indicating highly heterogeneous pore structures. The tortuosity fractal dimension decreases with increased porosity and pore fractal dimension. And enlarged pore size range can enhance tortuosity fractal dimension under certain pore fractal dimension. The present fractal model may help understanding the transport mechanisms of porous media and provide useful guideline for oil and gas exploitation, hydraulic resource development, geotechnical engineering and chemical engineering etc.

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Effective Thermal Conductivity of Saturated/Unsaturated Porous Media based on Fractal Geometry

Authors: Peng Xu[1]; Yuqing Shen[1]

Co-authors: Min Wang [1]; Shuxia Qiu [2]

[1] *China Jiliang University*

[2] *University of Shanghai for Science and Technology*

Corresponding Author: xupeng@cjlu.edu.cn

The effective thermal conductivity (ETC) is one of the most important thermo-physical properties for quantifying conductive heat transfer in saturated (two-phase) and unsaturated (three-phase) porous media. Evaluation of the effective thermal conductivity is essential to a lot of engineering applications such as thermally enhanced oil and gas recovery, geothermal energy, carbon dioxide sequestration, nuclear waste disposal, chemical and biological engineering, drying technology, phase change materials for thermal energy storage, thermoelectric materials, polymer composite molding, porous building materials etc. However, the existing models for effective thermal conductivity cannot realistically account for the complex pore structures and generally contain empirical parameters. Therefore, fractal dimensions for pore size distribution and capillary tortuosity are introduced to characterize the pore-scale structure, and a generalized model for the effective thermal conductivity of saturated/unsaturated porous media is developed based on thermal-electrical analogy. The proposed fractal model has been validated by comparing with available experimental data. The results show that the effective thermal conductivity gradually decreases with the increase of porosity and pore fractal dimension as well as tortuosity fractal dimension. And the effective thermal conductivity increases with the increase of liquid saturation as the thermal conductivity of solid and liquid phases are larger than that of gas phase. However, it is inversely proportional to liquid saturation as the thermal conductivity of solid and liquid phases are smaller than that of gas phase. All

the parameters in the proposed effective thermal conductivity model have specific physical meanings, and it may capture the microstructure characteristics and help understanding the heat transfer mechanisms in porous media.

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Migration and Residual Trapping of Immiscible Fluids during Cyclic Injection

Author: Sookyun Wang[1]

Co-authors: Minhee Lee [1]; Junggi Um [1]; Seon-Ok Kim [1]

[1] *Pukyong National University*

Corresponding Authors: heelee@pknu.ac.kr, sookyun@pknu.ac.kr, jum@pknu.ac.kr, seonok@pknu.ac.kr

Geological CO2 sequestration (GCS) is one of the most promising technologies for mitigating greenhouse-gas emission into the atmosphere. In GCS operations, residual trapping is the most favorable form of trapping mechanism because of its storage security and capacity. In this study, the effects of cyclic injection of CO2-water on the immiscible displacement and residual trapping in pore networks were examined. For the purpose, a series of injection experiments with five sets of drainage-imbibition cycles were performed using 2D transparent micromodels and a pair of proxy fluids, n-hexane and deionized water. The multiphase flow and immiscible displacement phenomena during drainage and imbibition processes in pore networks were visually observed, and the temporal and spatial changes in distribution and saturation of the two immiscible fluids were quantitatively estimated at the pore-scale using image analysis techniques. The results showed that the mobile region for invading fluids asymptotically decreased because the randomly-diverged flow paths created at early cycles converged to a fewer active flow paths over multiple cycles. They also showed that the immobile region, which were created by entangled tiny blobs of immiscible fluids in the residual phase, gradually increased as one fluid previously flooded as continuous steams were dispersed and isolated into numerous small-scale blobs by the other fluid newly invading. These processes repeated until the immobile region approached the main flow channels. The observations and analyses in this study implied that application of cyclic injection in GCS operations may be used to store large-scale continuous CO2 streams in small-scale dispersed forms, which may significantly improve the effectiveness and security of geological CO2 sequestration.

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Thermal coupled reactive transport in porous media based on SPH method

Author: Qianhong Yang[None]

Co-authors: Jun Yao [1]; Zhaoqin Huang [1]

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

Corresponding Authors: s17020254@s.upc.edu.cn, huangzhqin@upc.edu.cn

Surface reaction such as mineral precipitation and dissolution is a typical moving boundary problem with time dependent interface. Examples of this issue such as crystallization and reactive flow in porous media have been broadly studied due to the importance in natural and industrial field. The recent development of full Lagrangain methods provides a new way to simulate such dynamical process without requiring adaptive mesh and interface tracking techniques. Smoothed particle hydrodynamics is a typical Lagrangian, mesh-free method, which is quite suitable to simulate the above problem. The physical effect such as solute transport and thermal flow can be incorporated into the framework of SPH with relative ease. In the present work, crystallization and reactive transport in porous media together with the effect of thermal dynamics are investigated in the SPH framework. The new SPH version of discretized format of heat conduction equation is introduced and verified through benchmarks. The crystallization and reactive flow under different conditions are proposed in this study based on SPH simulation.

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GAS DIFFUSION COEFFICIENT OF FRACTAL POROUS MEDIA WITH ROUGH SURFACES BY MONTE CARLO SIMULATIONS

Author: Qian Zheng[None]

Gas diffusion behavior in fractal porous media with rough surfaces is simulated by Monte Carlo technique in this work. Based on the fractal character of pore size and its surfaces in porous media, the probability model of the effective gas diffusion coefficient is derived. The proposed model of the effective gas diffusion coefficient is explicitly expressed as a function of structural parameters of porous media, such as surface roughness, porosity, pore size, the fractal dimensions for pore area and tortuosity. The effect of structural parameters of porous media has been studied in detail. The results show that the present results from the Monte Carlo simulations present a good agreement with those from the available analytical model and the available experimental data. The proposed Monte Carlo simulation technique may have the potential in predictions of other gas transport properties in fractal porous media.

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Analysis of capillary imbibition for fluid through confined Nano pores

Authors: Fanhui Zeng[1]; Qiang Zhang[1]; Jianchun Guo[1]; Yu Zhang[1]

[1] *State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu, China*

Corresponding Authors: zhangyu0971@126.com, guojianchun@163.com, zq1819096@163.com, zengfanhui023024@126.com

The confined Nano pores spontaneous capillary imbibition is investigated using analytical model that includes the slip effect, wettability and effective viscosity at the water surface interface. Results show that the effective viscosity larger than that of bulk water, decrease with the diameter and wettability. The effective slip length is negative for the contact angle smaller than 90 degrees. However, for the contact angle larger than 90 degrees, the effective slip length is positive and increase with diameter. Results of the presented model shows that capillary imbibition length of Nano confined water can decrease up to 1.164 -1.644 times that calculated by the no-slip Lucas-Washburn equation for Nano pores due to effective viscosity and slippage with various dimensions and contact angles. The enhancement increases with diameter and contact angle. These results offer a new understanding of confined Nano pore fluids, which can be used to control fracturing fluid flow in the nanoscale shale reservoir formation.
Key words: Shale gas formation, Nano pores confined flow, Slippage, Wettability, Viscosity, Spontaneous imbibition

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Automatic well test interpretation based on convolutional neural network for infinite reservoir

Authors: Xuliang Liu[1]; Daolun Li [1]; Jinghai Yang [2]; Wenshu Zha [1]

[1] *Hefei University of Technology*

[2] *Daqing Oilfield Logging Technology Service Company*

Corresponding Authors: 13904599605@163.com, wszha@hfut.edu.cn, 2017111294@mail.hfut.edu.cn, ldaol@ustc.edu.cn

Abstract The well testing technique has been widely used to estimate well and reservoir parameters, such as permeability, skin factor and so on. For a long time, well testing interpretation has been conducted manually. Even though, traditional artificial neural networks (ANNs) was introduced as an automatic well test interpretation method, the results were disappointed. This paper proposes a new intelligent well test interpretation method based on convolutional neural network (CNN) for infinite reservoirs. In this method, the wellbore storage coefficient, skin factor and reservoir permeability are defined into a dimensionless group C_De^{2S}. The pressure change and pressure derivative in log-log plot are taken as the input of the CNN, and the corresponding dimensionless group $log\left(C_De^{2S}\right)$ is used as CNN's output. The optimized CNN is obtained by minimizing mean square error (MSE) of training data and mean relative error (MRE) over validation data. The Optimum CNN can directly apply to interpret the buildup or drawdown pressure for wells in infinite large reservoir. This new method is tested for its effectiveness and accuracy in Daqing oil field, China. It demonstrates that, for wells in infinite reservoir, CNN has superior learning capability than traditional ANNs and could be used as an automatic well test interpretation technique. Utilizing CNN for reservoirs with more complicated flow models will be our future work.
Keywords: well testing; convolutional neural network; automatic interpretation; infinite reservoir

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Permeability of salt crusts from evaporation of sand columns

Author: Joseph Piotrowski[1]

Co-authors: Johan Alexander (Sander) Huisman [1]; Andreas Pohlmeier [1]; Uri Nachshon [2]; Harry Vereecken [1]

[1] *FZ-Juelich (Juelich Research Centre), Germany*

[2] *Ben Gurion University of the Negev, Geology*

Corresponding Authors: h.vereecken@fz-juelich.de, s.huisman@fz-juelich.de, a.pohlmeier@fz-juelich.de, j.piotrowski@fz-juelich.de, urina@volcani.agri.gov.il

Salt precipitation due to evaporation leads to the formation of a salt crust that affects the flow and transport of water and solutes in the top layer of porous media with practical implications for a range of topics, including soil salinization, erosion and land loss, and damage to building materials. Many studies have investigated evaporation of saline solutions from porous media. However, little is known about the transport properties of developing salt crusts despite their importance for accurate modeling of evaporation. Recently, Nachshon et al. (2015) reported permeability estimates for two different types of salt crusts. In their approach, the permeability of a brine-saturated sample was determined first using a constant-head permeameter. Then, a salt crust was allowed to form by evaporation. After resaturation of the sample, the permeability of the sample with crust was determined again and the crust permeability was determined from the difference between the measured permeability with and without crust. Permeability determination using this approach is prone to inaccuracy due to air entrapment and mechanical deformation during resaturation. To circumvent these issues, the first aim of this study is to assess the convenience of a novel measurement approach to determine crust permeability based on a gas permeameter set-up. A second aim is to investigate differences in crust permeability for four commonly occurring salt types (NaCl, MgSO4, Na2SO4, and CaCl2). To achieve these aims, sand columns were saturated with brine solutions with an initial concentration of one third of the maximum solubility for each salt. The samples were wet packed in triplicates with F32 quartz sand (240 µm mean grain diameter) in plexiglass columns with a diameter of 31 mm and a filling height of 80 mm. All samples were allowed to drain before the bottom opening was closed to ensure that mass loss was due to evaporation from the surface only. Evaporation took place at 25 ℃ ± 1 ℃ and 0.25 ± 0.05 relative humidity and the water content of each sample was determined gravimetrically every day. After evaporation to a fixed relative degree of 30 % saturation, clear salt crusts formed on all samples. In order to determine the crust permeability, the sand below the crust was removed first. Subsequently, we measured the crust permeability using a gas-permeameter set-up based on Takeuchi et al. (2008). In this set-up, an N2 gas flux was flown through the porous crust at a known low flow rate and the pressure difference across the sample was measured in order to calculate gas permeability using Darcy's law (Ball et al., 2001). The results showed that the observed evaporation rates for the columns with different salt types initially varied according to the saturation pressure of the brine, but were differently affected by the establishment of a salt crust later in the experiment. This was attributed to differences in crust permeability of different salt types, which were found to vary by more than one order of magnitude depending on the type of salt and crust (efflorescent or subflorescent).

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Impact of fracture sealing on the percolation state of orthogonal fracture networks

Author: Weiwei Zhu[1]

Co-authors: Siarhei Khirevich [1]; TADEUSZ PATZEK [2]

[1] *King Abdullah University of Science and Technology*

[2] *KAUST*

Corresponding Authors: tadeusz.patzek@kaust.edu.sa, weiwei.zhu@kaust.edu.sa, khirevich@gmail.com

Natural fractures and their complex networks are ubiquitous in crustal rocks. Since fractures are far more permeable than the surrounding matrix, they have a significant impact on fluid flow in subsurface (Berkowitz, 2002). Orthogonal joint sets (mode I fractures) in particular, are topologically well-connected (Rives et al., 1994). However, hydraulic connectivity of topologically connected fractures is not guaranteed, because they can be sealed mainly due to in-situ compressive stress (Olson et al., 2007) and cementation (Lander and Laubach, 2015). Fracture sealing, as well as the impact of fractures on flow, have been extensively investigated as two separate research topics. However, the impact of fracture sealing on flow has been rarely studied before.

In this research, we apply a percolation approach (Stauffer and Aharony, 2014) instead of expensive flow simulations to investigate the impact of fracture sealing on the hydraulic connectivity of orthogonal fracture networks. From the percolation analysis, a hydraulically connected spanning cluster is identified. Confirmation of fracture connectivity is usually the ultimate purpose of engineering applications, since these fractures likely provide the highly permeable pathways for fluid flow.

We model the orthogonal fracture networks in both 2D and 3D. Fracture spacing is positively correlated with the formation thickness. Different spacing distributions, such as uniform distribution, lognormal distribution, and exponential distribution, are applied to describe each fracture set. To model sealed fractures, we divide each fracture into small segments and seal a given proportion of these segments. The impact of geomechanics and geochemistry on the degree and spatial distribution of sealing is considered to make our model more realistic and meaningful. For each set of the parameter values, we generate 100 realizations and check the corresponding percolation state individually. The impact of the matrix is neglected, since fractures dominate flow if their permeability is much higher than that of the matrix, e.g., five orders of magnitude higher, as suggested by our previous research.

From preliminary observations, we find that fracture sealing can prevent the formation of the spanning cluster, even with a small proportion of sealed fractures (5 to 10 per cent). The spacing distribution of each fracture set has a significant impact on the percolation state. A 3D fracture system is much easier to percolate than a 2D fracture system. Smaller fractures make it much harder for a spanning cluster to form. In general, fracture sealing essentially plays a negative role in hydraulic connectivity. For fracture networks that are not as geometrically well-connected as orthogonal networks, the impact is even more significant. This research emphasizes the importance of fracture sealing on hydraulic connectivity and provides a more complete picture of fracture networks in subsurface.

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A three-field approach for flow simulations in networks of fractures on non conforming meshes

Authors: Stefano Berrone[1]; Sandra Pieraccini[None]; Stefano Scialò[2]; Denise Grappein[2]

[1] *Politecnico di Torino, Italy*

[2] *Politecnico di Torino*

Corresponding Authors: stefano.berrone@polito.it, denise.grappein@polito.it, sandra.pieraccini@polito.it, stefano.scialo@polito.it

The present work proposes a new numerical strategy for the simulation of flows in the subsoil, described by means of the discrete fracture network (DFN) model. A DFN is a set of intersecting planar polygons resembling the fractures in the underground rock matrix. Simulations in DFNs for realistic applications are particularly challenging as a consequence of the complex, multi-scale nature of such domains. This strongly limits the applicability of standard numerical tools, mainly for the impossibility of generating good quality conforming meshes of such domains with a reasonable number of unknowns.
Recently, an approach based on the numerical optimization and non-confoming meshes has been proposed in order to effectively handle DFN flow simulations on large scales, completely overcoming any mesh-generation problem [1, 2]. A cost functional is introduced, expressing the error in the fulfillment of suitable matching conditions at the intersections between fractures and it is minimized constrained by the equations governing the flow on each fracture.
Here a new formulation of this approach is proposed, still based on the numerical optimization, but using a three-field formulation [3] for the description of the constraint equations. This produces a new scheme which retains the robustness to complex geometries, the capability of handling non-conforming meshes and the predisposition to parallel implementation of the previous approach, and introduces new characteristics: the new functional is mono-objective, thus simplifying the minimization process, and the new scheme is locally mass-conservative across fracture intersections.

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Numerical modeling of coupled heat and water transport for the study of permafrost dynamics: High Performance Computing simulations for watershed scale analysis

Authors: Laurent Orgogozo[1]; Oleg S. Pokrovsky[2]; Christophe Grenier[3]; Emmanuel Mouche[3]; Manuel Marcoux[4]; Michel Quintard[5]

[1] *GET (Géosciences Environnement Toulouse), UMR 5563 CNRS / UR 234 IRD / UPS, Observatoire Midi-Pyrénées, Université de Toulouse, 14 avenue Édouard Belin, 31400 Toulouse, France*

[2] *GET (Géosciences Environnement Toulouse), UMR 5563 CNRS / UR 234 IRD / UPS, Observatoire Midi-Pyrénées, Université de Toulouse, 14 avenue Édouard Belin, 31400 Toulouse, France - BIO-GEO-CLIM laboratory, Tomsk State University, Lenina 35, Tomsk, Russia*

[3] *Laboratoire des Sciences du Climat et de l'Environnement, Université Paris-Saclay, IPSL / LSCE, UMR 8212 CNRS-CEA-UVSQ, Orme des Merisiers, 91191 Gif-sur-Yvette Cedex, France*

[4] *Université de Toulouse, INPT, UPS, IMFT (Institut de Mécanique des Fluides de Toulouse), Allée Camille Soula, F-31400 Toulouse, France*

[5] *Université de Toulouse, INPT, UPS, IMFT (Institut de Mécanique des Fluides de Toulouse), Allée Camille Soula, F-31400 Toulouse, France - CNRS, IMFT: F-31400 Toulouse, France*

Corresponding Author: laurent.orgogozo@get.omp.eu

Permafrost is year round frozen soil, which covers 25% of the land of the northern hemisphere. The presence of permafrost affects tremendously both the natural processes (e.g.: water cycle) and the human activities (e.g.: building) in the affected areas. Its dynamics is governed by strongly coupled heat and mass (mainly water) transport, with couplings related for instance to advective transport of heat by water fluxes or to the strong impacts of phase changes on the hydrodynamic properties of soils. Moreover, these physical phenomena are affected by numerous non-linearities. Although challenging, the numerical simulation of coupled heat and mass transport in permafrost is needed both for environmental science and for cold regions engineering. The modeling of active (unfrozen) layer processes or the evaluation of climate-induced or technogenic permafrost thaw are classical applications of such numerical simulations. One of the major difficulties that limits the applicability of this kind of modeling is the huge computational resources that may be needed due to the strong non-linearities and couplings of the considered physical phenomena. This problem is especially critical for large scale 3D applications such as experimental watershed modeling. For this kind of studies the use of High Performance Computing (HPC) softwares and facilities is required. Here we present the first 3D thermo-hydrological simulation of a permafrost affected catchment performed with the massively parallel solver permaFoam, the OpenFOAM® solver for permafrost modeling. The conservation equations solved by permaFoam govern the 3D transient transport of water and heat in variably saturated porous media, taking into account freeze/thaw cycle of the pore water and water uptake in the root layer associated to evapotranspiration (Orgogozo et al., 2019). This solver has been implemented in the open source, generalist Computational Fluid Dynamics (CFD) tool box OpenFOAM®, so that it can benefit from the good parallel performances of this well-known HPC software. First a brief introduction of the permaFoam solver will be done, describing the implementation choices, the associated underlying assumptions and the adopted validation strategy. Then a case study dedicated to the characterization of the multi-decadal evolution under climate change of the thermo-hydrological state of a 40 km2 experimental catchment of Central Siberia will be presented. The related computations have been performed on regional (Olympe, ~13 000 cores, CALMIP) and national (Occigen, ~80 000 cores, CINES) supercomputers, and we will make a focus on the associated numerical challenges, such as scalability issues and I/O's handling. Finally, the perspectives associated to these numerical developments will be discussed.

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Upscaling Diffusive Transport in Terms of Porosity Statisitcs

Authors: Alraune Zech[1]; Matthijs de Winter[1]

[1] *Utrecht University*

Corresponding Authors: d.a.m.dewinter@uu.nl, a.zech@uu.nl

Gas diffusion is the rate limiting transport mechanisms in fields such as preparative chromatography and heterogeneous catalysis. The transport rate is limited by the available pore space, in particular at low porosities. Typically, pores facilitating diffusion are of the order of 1 nm up to several micrometers in diameter, which require sophisticated visualization techniques such as electron microscopy to be able to decipher the pore space. Resolving the pore space with high spatial resolution has the disadvantage that it can only probe small volumes, often below a representative elementary volume (REV). Meanwhile, heterogeneity of the pore space may occur across larger length scales.
We have investigated the statistics of transport abilities of volumes smaller than a REV as a function of porosity and percolation probability. The initial statistics are based on a fluid catalytic cracking particle. We determined a probability distribution function for the transport ability as a function of porosity. Furthermore, we investigated the effect of upscaling the probability distribution function, with special focus on sub-REV volumes. The analytical results are compared to pore network-type simulations. We believe that the statistics-based up-scaling technique of sub-REV microscopy data provides a new tool in understanding macroscopic transport behavior of micro-porous materials.

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The effect of salinity on fecal bacteria transport through porous media

Authors: Dong Zhang[1]; Valentina Prigiobbe[1]

[1] *Stevens Institute of Technology*

Corresponding Authors: vprigiob@stevens.edu, dzhang18@stevens.edu

The reuse of wastewater in agricultural is a common practice worldwide, in particular in arid and semiarid regions. However, untreated or partially treated wastewater may contain excessive concentration of fecal bacteria that can enter surface water bodies and groundwater systems pose a risk to human health [1,2]. Therefore, it is important to understand the fate of fecal microorganisms in soil. The fate and the transport of fecal bacteria in soil is governed by attachment and detachment processes at the solid-liquid interface, which are controlled by the soil properties and the chemical composition of the solution. The salinity (or ionic strength) is one of the most important factor as it controls the electrostatic interactions between the bacteria and the porous medium surface and, therefore, the speed of their migration. Salinity can be significant in untreated or partially treated wastewater. At high salinity, the attachment of bacteria onto a porous medium surface is the dominant process. However, few studies [3,4] quantitatively analyze the effect of the salinity on the transport behavior of bacteria in porous media. Moreover, these studies do not account for the coupling of the bacteria and salinity, which is evident from experimental observations. Missing therefore the possibility to describe the effect of the variations of salinity with their models.

Here, a study is presented which combines laboratory tests with modeling. It was carried out to understand the role of salinity on fecal bacteria transport in porous media. Column-flood experiments were conducted to investigate the transport of the bacteria through sand and they were continuously monitored with UV-Vis spectrometer. One dimensional transport model was developed and used to describe the experiments [5]. The model consists of two mass conservation equations of the bacteria and the salt concentration coupled through the constitutive equations of attachment/detachment process. The results show that under salinity reduction, a peak of bacteria concentration forms, which is instead not predicted by the classical models. The magnitude of the peak is controlled by the detachment process and the pore size. Overall, this work helps to gain an insight into the understanding of the effect of salinity gradients and pore size on fecal bacteria transport which may occur during wastewater reuse in agricultural soil.

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Carrying nanoparticles through porous media using foam for contaminated site remediation

Authors: Qingjian Li[1]; Valentina Prigiobbe[1]

[1] *Stevens Institute of Technology*

Corresponding Authors: vprigiob@stevens.edu, qli39@stevens.edu

Wet foam is a complex fluid consisting of bubbles dispersed into a liquid phase, with a volume fraction of the gas phase up to 97 vol.%.
Nanoparticles have been used to stabilize bubbles. They can adsorb at the gas-liquid interface providing remarkable stability to the foam. This phenomenon opens the opportunity of carrying nanoparticles through porous media using foam and a promising application is in the remediation of contaminated sites. The foam helps to overcome the major challenges of nanoparticle transport, namely, mobility control, aggregation, and retention.
However, the transport of nanoparticles with foam cannot be described with the current models; as the mechanisms of particle-bubble interaction during transport in porous media are not well understood, yet.

Here, a modeling and experimental work are presented where nanoparticles made of silica and nano zero-valent iron (nZVI) and transported with trough a medium made of sand are tested and described. Experiments at the pore-scale with 2D porous media chip were carried out and the constitutive equation for foam generation in the presence of nanoparticles formulated and combined with a mathematical model for nanoparticles and foam transport. Anionic and cationic surfactants combined with bare silica and nZVI nanoparticles were used to stabilize a foam made of air. Overall, the results show that the foam generation mechanism is not affected by the presence of nanoparticles and that a foam significantly enhances the efficiency of nanoparticle delivery. Moreover, the developed

mathematical model agrees very well with experimental observations.
In conclusion, this work suggests that foam can be a valuable alternative to conventional methods to deliver nanoparticles in the subsurface in an efficient and sustainable manner, given the negligible amount of water required.

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Three-dimensional characterization of pore space architecture in granular materials

Author: Nimisha Roy[1]

Co-author: David Frost [1]

[1] *Georgia Institute of Technology*

Corresponding Authors: david.frost@ce.gatech.edu, nroy9@gatech.edu

The characterization of the pore space geometry in granular material microstructure constitutes the basis for prediction and analysis of macro-scale constitutive relationships and accurate modelling of transport phenomena through porous media. More specifically, the interplay between pore and throat geometries governs fluid flow characteristics like turbulence in multiphase flow, wetting characterization, viscous fingering and snap-off. Classical pore models generally assume simplified pore and throat geometries, comprised of spherical pores connected by prismatic tubes of constant cross-section. This is largely due to the lack of computational tools necessary to adequately characterize the complex pore space architecture. This paper presents a new geometrical approach to partition the pore space of granular material microstructure into a three-dimensional network of pore bodies interconnected by pore throats, without inherent assumptions about their geometries. The algorithm allows the extraction of parameters like the three-dimensional size and shape of pore bodies, throats and constriction surfaces (narrowest cross-section of a throat) along with the sharpness of the pore throats. The proposed method is validated against simulated idealized packed structures of known pore geometries and is demonstrated on synthetic packed particle systems and reconstructed sand microstructures.

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Three-dimensional characterization of pore space architecture in granular materials

Authors: Nimisha Roy[1]; David Frost[1]

[1] *Georgia Institute of Technology*

Corresponding Authors: nroy9@gatech.edu, david.frost@ce.gatech.edu

The characterization of the pore space geometry in granular material microstructure constitutes the basis for prediction and analysis of macro-scale constitutive relationships and accurate modelling of transport phenomena through porous media. More specifically, the interplay between pore and throat geometries governs fluid flow characteristics like turbulence in multiphase flow, wetting characterization, viscous fingering and snap-off. Classical pore models generally assume simplified pore and throat geometries, comprised of spherical pores connected by prismatic tubes of constant cross-section. This is largely due to the lack of computational tools necessary to adequately characterize the complex pore space architecture. This paper presents a new geometrical approach to partition the pore space of granular material microstructure into a three-dimensional network of pore bodies interconnected by pore throats, without inherent assumptions about their geometries. The algorithm allows the extraction of parameters like the three-dimensional size and shape of pore bodies, throats and constriction surfaces (narrowest cross-section of a throat) along with the sharpness of the pore throats. The proposed method is validated against simulated idealized packed structures of known pore geometries and is demonstrated on synthetic packed particle systems and reconstructed sand microstructures.

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Effect of Wetting Transition during Multiphase Displacement in Porous Media

Authors: Zhongzheng Wang[1]; Jean-Michel Pereira[2]; Yixiang Gan[1]

[1] *The University of Sydney*

[2] *École des Ponts ParisTech*

Corresponding Authors: yixiang.gan@sydney.edu.au, zwan4662@uni.sydney.edu.au, jeanmichel.pereira@enpc.fr

The effects of wettability on multiphase displacement in porous media have been studied extensively in the past, and the contact angle is identified as an important factor influencing the displacement patterns. At the same time, it has been found that effective contact angle can vary drastically in a time-dependent manner on rough surfaces due to Cassie-Wenzel wetting transition. In this study, we develop a theoretical model at the pore scale describing the apparent contact angle on rough interface as a function of immersed time. The theory is then incorporated into the Lattice Boltzmann method for simulating multiphase displacement in disordered porous media. A dimensionless time ratio, Dy, describing the relative speed between the wetting transition and pore invasion is defined. We show that the displacement patterns can be significantly influenced by Dy, where more trapped defending ganglia can be observed at large Dy (i.e., a relatively slow wetting transition process), leading to lower displacement efficiency. We investigate the mobilisation of trapped ganglia through identifying different mobilisation dynamics during displacement, including translation, coalescence, and fragmentation. Agreement is observed between the mobilisation statistics and the total pressure gradient across a wide range of Dy. Understanding the effect of wetting transition during multiphase displacement in porous media is of importance for applications such as carbon geosequestration and oil recovery, especially for most porous media that solid surface roughness cannot be neglected.

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A multi-scale diffuse interface/front tracking model for multi-component two-phase flow

Authors: Guangpu Zhu[1]; Kou Jisheng[2]; Yao Jun[3]; Qianhong Yang[4]

[1] *Research Center of Multiphase Flow in Porous Media, China University of Petroleum (East China)*

[2] *Shaoxing University*

[3] *Research Center of Multiphase Flow in Porous Media*

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

Corresponding Authors: s17020254@s.upc.edu.cn, zhugpupc@gmail.com

In this work, we use a diffuse interface/front tracking model to simulate multi-component two-phase flow with partial miscibility based on a realistic equation of state (e.g. Peng–Robinson equation of state). Because of partial miscibility, thermodynamic relations are used to model not only interfacial properties but also bulk properties, including density, composition, pressure, and realistic viscosity. In the numerical simulation, we use a multi-scale simulation method to resolve the high contrast of scales from the microscopic interface composition to macroscale bulk fluid motion since the interface has a nanoscale thickness only. At the microscopic scale, we consider the partial miscibility of multiple components and calculate the capillary pressure base on the assumption of thermodynamic equilibrium. At the macroscopic scale, the interfaces are treated as discontinuous surfaces separating two phases of fluids, and the front tracking method is adopted to tracking the interface. The generalized Navier boundary condition is adopted to consider the moving contact line problem at the solid surface. Using the multi-scale diffuse interface/front tracking model, we investigate the flow dynamics of shale oil in porous media.

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Dealing with Model Uncertainty and Deficiencies in Thermal Breakthrough Models

Authors: Anna Suzuki[1]; Elvar K. Bjarkason[1]

[1] *Institute of Fluid Science, Tohoku University*

Corresponding Authors: e.bjarkason@tohoku.ac.jp, anna.suzuki@tohoku.ac.jp

Thermal breakthrough models are simplified representations of thermal and fluid transport processes occurring within geothermal systems which consist of hot, fractured porous rocks. Since simple thermal breakthrough models only require modest computational resources and are easy to use, they are widely adopted in practice to describe observed temperature changes in geothermal fields. However, those models have various model deficiencies (model errors), which can severely impact uncertainty estimates and model predictions. This study considers methods for enhancing estimates of model predictive uncertainties for thermal breakthrough models used to model temperature changes in geothermal fields. To account for or soften the effects of model errors, we use a total observation error covariance matrix. This total covariance matrix is used to account for both model errors as well as observation errors, which like the model errors might be underestimated initially by the model developers. For estimating model parameter uncertainty, we apply an ensemble smoother and update the total covariance matrix iteratively based on the posterior ensemble of observation residuals given by the ensemble smoother. We applied the total covariance approach to geothermal field data from two different sites. The results suggest that the total covariance approach can provide better thermal breakthrough predictions for real geothermal field studies. The total covariance scheme gives wider predictive temperature intervals than those found when neglecting model

errors. Consequently, the total covariance approach gives a better portrayal of potential future temperature changes. In conjunction with the total covariance approach, we, additionally, discuss the importance of refining imperfect thermal breakthrough models to improve model predictions under uncertainty.

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An efficient stochastic simulation of shale gas development based on deep learning algorithm

Authors: Liang Xue[1]; Junru Zhang[2]

[1] *China University of Petroleum*

[2] *China University of Petroleum (Beijing)*

Corresponding Authors: 2018212177@student.cup.edu.cn, xue_liang1983@163.com

Abstract Shale gas is one of the major unconventional energy resources, and it is critical to predict shale gas production capacity accurately so that a reasonable development strategy can be made under uncertainty. Shale gas reservoir has the characteristics of ultra-low permeability, multi-scale gas flow mechanism and complex hydraulic and natural fracture system. The data to characterize the shale gas natural fracture system are very limited, which leads to high uncertainty of the model. The stochastic simulation based on Monte Carlo method requires a huge amount of calculation efforts to characterize the saturation distribution of shale gas reservoir under uncertainty. Surrogate strategies are used widely for uncertainty quantification in order to improve computational efficiency. In this paper, we propose a deep convolutional neural network methodology to simulate shale gas development process stochastically. The aim of the proposed deep learning method is to transform the shale gas saturation prediction problem into an image-to-image regression strategy. A set of natural fractures are randomly generated according to the statistical information obtained from well logging and outcrops. The embedded discrete fracture model (EDFM) is used to simulate the production of shale gas reservoir under different natural fracture distribution conditions, and the saturation distribution of gas reservoir can be obtained. The deep learning method takes the natural fracture distribution (or its equivalent permeability distribution) as input and shale gas saturation distribution as output. After the training process, the deep learning method can build a relationship between permeability distribution and its corresponding saturation distribution, which can be used as the surrogate in the consequent stochastic simulation process. The results show that the deep learning surrogate model can be sufficiently accurate to characterize the predictive uncertainty and remain computationally efficient compared to numerical simulation.

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Pore Scale Study of Solid/Liquid Phase Change in a 3D Cubic Lattice Metal Frame

Author: Chunyang Wang[1]

Co-author: Moghtada Mobedi [1]

[1] *Shizuoka University*

Corresponding Authors: moghtada.mobedi@shizuoka.ac.jp, 627351102@qq.com

A numerical study on solid/liquid phase change in a 3D cubic metal frame is performed. The computational domain consists of 125 cells and each cell is fully filled with PCM (Phase Change Materials). For the pore scale study, the continuity, momentum and energy equations are solved for the liquid phase by using enthalpy method while the heat conduction equation is used to find out temperature in the solid phase. Based on the obtained temperature field, the interfacial heat transfer coefficient between the solid and fluid phases is calculated. For the volume average study, the volume averaged continuity, momentum and energy equations are solved for the solid and fluid phases, and the volume averaged temperature field is obtained.
In this study, firstly a discussion is done on the change of the obtained interfacial heat transfer coefficient for the entire domain during the melting process. Secondly, the comparison of the volume averaged temperature with the pore scale results are done, and finally the accuracy of the correlation employed in literature for heat transfer coefficient is investigated. The study is performed for two different values of porosity as 0.9 and 0.5 when the Raleigh and Stefan numbers are equal to 106 and 0.6, respectively. All results and discussions are supported by 3D isotherms and velocity vector fields. A good agreement for the temperature and velocity distributions between pore scale and volume average results are observed, particularly for the local thermal equilibrium case when the porosity is 0.9. It is observed that, the interfacial heat transfer coefficient between the solid and fluid phases are not constant and has a pick during the phase change.

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Fluid flow through anisotropic and deformable double porosity media with ultra-low matrix permeability: An efficient continuum framework

Authors: Qi Zhang[1]; Ronaldo Borja[1]

[1] *Stanford University*

Corresponding Authors: borja@stanford.edu, qzhang94@stanford.edu

Fractured porous media or double porosity media are common in nature while efficient modeling still remains a significant challenge due to bimodal pore size distribution, anisotropy, multi-field coupling and various flow patterns. The purpose of this study is to formulate an efficient coupled flow and geomechanics model of anisotropic and deformable double porosity media with ultra-low matrix permeability. Fluid flow in fissures is modeled with generalized Darcy's law with permeability conceptually upscaled from detailed geological characterizations while fluid flow in much less permeable matrix follows a low velocity non-Darcy flow characterized by threshold value and nonlinearity, and fluid mass transfer is dependent on constant shape factor, fissure spacing, phase pressure difference, and analogous variable interface permeability. The geomechanics relies on a thermodynamically consistent effective stress derived from energy balance equation, and it is modeled following linear poroelastic theory. Scaling analysis is performed to drop negligible force density terms under reasonable parameters' ranges which also guarantee no violation of entropy inequality. Even though this study is motivated by shale properties, the discussion revolves around generic double porosity media. Numerical simulations of initial boundary value problems reveal the capability of this efficient framework to capture the crucial role of coupling, anisotropy and ultra-low matrix permeability in dictating the pressure and displacement fields.

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Evaluation of machine learning methods for predicting the oil-water relative permeability: a comparison of tuning processes and model performances

Authors: Baosheng Jiang[1]; Zhixue Sun[1]

[1] *Research Center of Multiphase Flow in Porous Media , China University of Petroleum (East China)*

Corresponding Authors: s18020121@s.upc.edu.cn, upcszx@upc.edu.cn

Relative permeability has a major role in reservoir simulation, history matching, and other sensitive tasks related to reservoir. Some scholars have proposed several empirical models to predict relative permeability for some special rock/fluid characteristics. However, these existing methods are expensive, time-consuming and inapplicable to a wider range of rock-fluid systems. Based on these disadvantages, an inexpensive, rapid and robust model is inevitable to determine oil/water relative permeability. In this paper, we evaluate five typical machine learning methods, namely Support Vector Machine Regression, Artificial Neural Network, Random Forest Regression, Gradient Tree Boosting Regression and Adaboost Regression for predicting the two-phase oil/water relative permeability using data from the open literature. The dataset is comprehensive, which including 1172 experimental points collected from published literature. Through the elbow method to select the best K value, and then the K-means clustering algorithm is used to identify and eliminate the abnormal data. The input to each model consists of temperature, oil viscosity, water saturation, and the absolute permeability. In this research, we utilized validation curve to determine the parameter search range and adopted the hyper-parameter optimization method to obtain the best parameter set for each model. The performance of each regression is also evaluated using coefficient of determination, root mean square error, and average absolute error. The statistical analysis of the obtained five machine learning methods for prediction of relative permeability demonstrated that ensemble methods are good algorithm choices for supervised regression of relative permeability. The Adaboost Regression is robust to overfitting and high precision because that model can adjust the corresponding weight of each sample and training multiple weak regression models, then combining the different weight weak regression models to form a final strong regression model. The comparison between the performance of the five machine learning methods and other empirical relative permeability models proves that Adaboost Regression is more robust, accurate and reliable for estimating the oil and water relative permeability.

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The influence of porosity and gas hydrate on tortuosity in porous media based on CT scanning - lattice Boltzmann method

Authors: Lei Liu[1]; Zhixue Sun[1]

[1] *China University of Petroleum*

Corresponding Authors: upcszx@upc.edu.cn, upcliulei@foxmail.com

Mineral resources such as petroleum and natural gas hydrates are all present in porous media. It is essential to understand the penetration channels of fluids in porous media in order to efficiently develop mineral resources. The tortuosity is often used to present the curve of the percolation channels in porous media and is an important parameter for characterizing the transport properties of porous media. In order to investigate the effect of porosity and hydrate morphology on the anisotropy of tortuosity respectively, the porous media obtained by CT scanning with a porosity range of 0.365~0.778 were selected and two types of gas hydrate were randomly generated in a selected porous media, include pore-filling and grain-coating. The lattice Boltzmann method was used to flow simulation and the tortuosity value was obtained. The results show that the tortuosity variation is sensitive to the porosity and hydrate morphology in porous media. A model is presented to measure the tortuosity of in porous media. The nonlinear function relationship between the tortuosity and the porosity is fitted and the value of the tortuosity decreases as the porosity increases. The magnitude of the tortuosity in the X direction is greater than that of the Y direction. That is the flow path of the fluid in the X direction is more tortuous. In addition, the formation of hydrate makes the fluid flow more complicated in porous media. The relationships between tortuosity and hydrate saturation are proposed to describe tortuosity variation. The variation of tortuosity of Grain-coating hydrate is more significant than that of pore-filling hydrate.

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Study on Water Quality Sensitivity and Characterization of Permeability in Water Flooding Sandstone Reservoirs

Authors: Xiankun SONG[1]; Jianzhong WANG[1]

[1] *Research Center of Multiphase Flow in Porous Media, China University of Petroleum (East China)*

Corresponding Authors: wangjzh@upc.edu.cn, 1292860438@qq.com

Water injection is one of the most commonly used development methods in a sandstone reservoir. The quality of water injection is the main factor affecting the effect of water injection development. The suspended solid particles, oil, bacteria and other pollutants in the water will block the pores of the rock, resulting in the slow decline of reservoir permeability, which cannot be ignored for the long-term oil field. According to the development history of the oil field, the sandstone cores with different permeability are studied experimentally. Combined with the relevant water quality recommendation standard (SY/T 5329-2012), the influence experiment of permeability of different

reservoirs with the increase of dimensionless injection quantity under five dissimilar water quality is designed, and the change rule between permeability retention rate and different water quality and dimensionless injection quantity is analyzed, and the concept of permeability water quality sensitivity is put forward. Through theoretical derivation, the mathematical expression describing permeability attenuation law is established, which can be used to predict and calculate the damage degree of current formation permeability, solve the matching problem of water quality and permeability, and improve the adaptability of water injection to the reservoir. This provides a theoretical basis for choosing water quality and improving the waterflood development effect of the sandstone reservoir.

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Hierarchical modeling of Hydro-mechanical Coupling in Fractured Shale Reservoirs with Multiple Porosity Scales

Author: Xia Yan[None]

Co-authors: Dongyan Fan [1]; Zhaoqin Huang [2]; Lijun Liu [3]; Jun Yao [4]

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

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

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

[4] *Center of multiphase flow in porous media, China University of Petroleum(East China)*

Corresponding Authors: liulijunupc@163.com, huangzhqin@upc.edu.cn, jsyanxia1989@163.com

This paper describes a hierarchical approach to simulate the hydro-mechanical coupling in the fractured shale reservoirs with multiscale pore structure, including kerogen and inorganic matter at microscopic scale, natural fractures at mesoscopic scale, and hydraulic fractures at macroscopic scale. Specifically, inorganic matter and kerogen are first homogenized to obtained the equivalent mesoscopic model, then it combined with natural fractures is further homogenized to obtained the equivalent macroscopic model, while hydraulic fractures are modeled explicitly by using the Embedded Discrete Fracture Model (EDFM). After that, the mixed space discretization (i.e., Mimetic Finite Difference (MFD) method for flow and stabilized eXtended Finite Element Method (XFEM) for geomechanics) and modified fixed stress sequential implicit methods are applied to solve the proposed model. Finally, we demonstrate the accuracy and application of the proposed method to capture the coupled hydro-mechanical impacts of multiscale pore structure on fluid flow in fractured shale reservoirs.

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A revisited compositional 2-phase flow model for gas transport at various scales in heterogeneous porous structures in a deep geological radioactive waste disposal facility

Author: Zakaria SAÂDI[1]

Co-authors: Abdellah AMRI [1]; Rachid ABABOU [2]

[1] *Institut de Radioprotection et de Sûreté Nucléaire (IRSN)*

[2] *Institut de Mécanique des Fluides de Toulouse (IMFT)*

Corresponding Authors: ababou@imft.fr, zakaria.saadi@irsn.fr

There is a considerable challenge in modelling gas transport at different (spatial-time) scales in the saturated-unsaturated heterogeneous porous structure of a deep geological high-level radioactive waste disposal facility (HLW-DF). Inconsistencies in the conceptual physical two-phase flow models and uncertainties in the input parameters of such models (lack of knowledge, spatial variability⋯) can lead to misunderstanding of physical phenomena occurring in a HLW-DF, which may affect its performance during the post-closure phase. Therefore, there is a need for developing new physical approaches, and to account for uncertainties, in order to enhance the mathematical modelling of compositional two-phase flow models applied to gas migration in a HLW-DF.

The purpose of this work is twofold: (i) to study the sensitivity to gas entry pressure, as a parameter in the hydraulic properties of clay-based materials, on the modelling of gas transport in a state of near full water saturation, and (ii) to analyze the propagation of uncertainty of the input parameters of gas transport models at various scales. Based on the codes iTOUGH2 (Finsterle et al., 2007) and TOUGH2-MP (Zhang et al., 2008), three test problems are studied in this work.

The first test problem is based on a 2-phase flow experiment carried out during 1.5 years in a deep borehole inside the Callovo Oxfordian (COx) clay rock, located in the Andra's underground laboratory (De La Vaissière, 2011). This modelling study reveals that the gas-entry pressure plays an important role in this experiment. This was demonstrated by an optimal fit of the hydraulic parameters of the van Genuchten-Mualem model (modified by Vogel et al., 2001). The least squares optimization was carried out through a single objective function, using measured points of water retention and of relative permeability (to gas and water) vs. capillary pressure in the COx clay rock.

The second test problem consists in the simulation of gas migration in a "module"composed of hundreds of waste cells, in a HLW-DF during 100 000 years. The heterogeneous porous structure in each waste cell is modeled in detail (host rock, EDZ, bentonite, concrete, backfill⋯). Simulations are run with zero and non-zero gas entry pressure to show the impact of this parameter to gas pressure inside the access drifts and main drift of the facility.

Finally, the third test problem consists in an application of uncertainty propagation methods in order to assess the uncertainty of model predictions due to input parameters uncertainty. Simulation results of gas and water fluxes during 100 000 years are presented using a simplified model of hydrogen migration in a HLW-DF (Saâdi et al., 2018), with appropriate probability density functions for the uncertain parameters (including the hydrogen source term, gas-entry pressure, intrinsic permeability and porosity).

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3D printing micro-model and deep learning method application for micro displacement experiment and remaining oil analysis

Author: Yimin Zhang[1]

Co-authors: Chengyan Lin [1]; Lihua Ren [1]; Yuqi Wu [1]

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

Corresponding Authors: wuyuqi150348@163.com, ycdzycmsi@126.com, renlh@upc.edu.cn, b18010036@s.upc.edu.cn

Most water flooding reservoirs have entered a high water cut period in China. At this stage, the study of the formation mechanism and distribution pattern of microscopic remaining oil is the basis for further potential exploitation of remaining oil.
As we all know, micro-displacement experiment is an effective method to study microscopic remaining oil, and the micro-model is the core component of the experiment. At present, microfluidic models have developed a variety of manufacturing methods, but they are mostly limited to two-dimensional planes, which are still quite different from the three-dimensional pore network of actual reservoirs.
Therefore, in this paper , 3D printing technology was applied to make the microscopic models based on the reservoir grains model extracted from μ-CT data to make up for the lack of spatial information of the two-dimensional model. The printing adopted stereolithography(SLA) technology and highly transparent photosensitive resin material, which had realized dynamic visual observation and image acquisition throughout the experimental process.
The microscopic model was used in the displacement experiment under 25℃ and 0.1MPa. Three pore structure types, two displacement methods (water flooding and ASP flooding) and three displacement rates were designed to study the formation mechanism and distribution pattern of microscopic remaining oil. A smart camera was used to collect images in the whole process of the experiment. After each experiment, the models were cleaned thoroughly for reuse. After that, computer image processing technology was used for the qualitative analysis of experimental images. It divided 6 types of remaining oil, such as flow around, cluster, dispersed oil drop, retention, oil film and corner shape. Convolutional neural networks were used to train models to achieve automatic identification and quantitative statistics of microscopic remaining oil types. This study hopes to provide a new idea for the experimental research and analysis of microscopic remaining oil, and it can be combined with numerical simulation methods (e.g. efinite element method, finite volume method) to study the law of fluid in porous media at the micro scale , which is also our future research content.
This research is a preliminary exploration of the application of 3D printing technology and deep learning methods to micro-remaining oil research. But there are still many shortcomings, such as: the temperature and pressure resistance of micro-models have not been well solved and the printing accuracy of micro-models still needs to be improved, which are also our future improvement direction.

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Upscaling capillary pressure functions for modeling vertical migration of CO2 in brine aquifers

Authors: Kan Bun Cheng[1]; Avinoam Rabinovich[1]

[1] *Tel Aviv University*

Corresponding Authors: kbcheng@gmail.com, avinoamr@tauex.tau.ac.il

Accurate modeling of CO2 migration following injection into an aquifer is paramount for CO2 storage projects. One of the important processes that must be properly accounted for is capillary trapping. This is extremely difficult when coarse grid blocks are used in simulations, since capillary trapping is directly related to permeability heterogeneity, which is significantly reduced in upscaling. Nevertheless, using fine scale models is not feasible due to the computational cost and therefore upscaling methods must be developed. While there is much literature on permeability and relative permeability upscaling, much less exists for capillary pressure (Pc). However, for gravity-capillary vertical migration, upscaling of Pc functions is crucial as it determines whether trapping will be modeled accurately.

In this study, various fine scale models of CO2 migration are considered. CO2 is initially injected at the bottom of an aquifer and then, after injection is stopped, it migrates due to influence of buoyancy and capillary pressure until equilibrium is reached. We show that for most problems, existing upscaling methods for Pc result in significant underestimation of CO2 trapping. Particularly, capillary limit upscaling, which is widely used, leads to extremely large errors in coarse scale simulations. We then propose to determine upscaled Pc by optimization, i.e., conducting coarse simulations iteratively to match saturation distribution of the fine scale solution. We learn from the optimization method of upscaling that the problem is in fact quite involved, requiring many fitting parameters to arrive at reasonably accurate upscaled simulations. While the new method is computationally demanding, it is the only one we have found that leads to accurate results. Furthermore, we show that the upscaled Pc functions can be reused in other realizations of the permeability field, provided that these have the same statistical characteristics (mean, log variance and correlation length). This indicates that the optimization upscaling may be useful in real-field cases.

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PEM fuel cell performance studies of a tree-like pattern milled on graphite flow field plates

Authors: Marco Sauermoser[1]; Signe Kjelstrup[1]; Natalya Kizilova[2]; Bruno G. Pollet[3]

[1] *PoreLab, Department of Chemistry, Norwegian University of Science and Technology, NTNU, Trondheim, Norway*

[2] *Institute of Aviation and Applied Mechanics, Warsaw University of Technology, Warsaw, Poland*

[3] *Department of Energy and Process Engineering, Norwegian University of Science and Technology, NTNU, Trondheim, Norway*

Corresponding Authors: bruno.g.pollet@ntnu.no, nkiz@meil.pw.edu.pl, signe.kjelstrup@ntnu.no, marco.sauermoser@ntnu.no

The ever challenging technical targets (see US DoE [1]) for Proton Exchange Membrane (PEM) fuel cells in terms of cost, performance, power density and durability, have created the need of better and more optimised flow field (FF) designs for flow field plates (FFP). In 2002, Morgan Fuel Cell Ltd (no longer trading) developed and patented a high-performance FF design called Biomimetic™, which was inspired from animal lungs and plant tissues [2]. Since then, other studies have shown that using such a design could increase PEM fuel cell performance [3,4]. For example, Bethapudi et al. [3] and Trogadas et al. [4] have recently shown that using FF patterns which are based on biological flow networks, like tree-shaped patterns, can increase the fuel cell performance [3,4]. Based on the work of Sauermoser et al. [5], a two-layer flow field plate has been developed, which possesses a tree-like flow pattern for both the inlet and outlet patterns. The patterns were milled on Schunk graphite plates by CNC machining performed by HySA Systems Competence Centre (University of the Western Cape, South Africa). The outlet and inlet ports were not directly connected, allowing for uniform fuel and oxidant distribution. The PEM fuel cell performance of the newly designed FF patterns of different scaling parameters for the inlet and outlet were investigated on a 25cm2 membrane

electrode assembly (MEA) active area. IV-curves, power curves and impedance spectra were generated at 70%, 60% and 50% relative humidity (RH) on both the Anode and Cathode using a Biologic FCT-50s PEMFC test station and a Baltic Fuel Cell qCF FC25 housing. PEM fuel cell performance data were compared to those obtained for a conventional 1-channel FF serpentine design.

Acknowledgement:
The authors are grateful to the Research Council of Norway through its Centres of Excellence funding scheme, project number 262644, PoreLab.

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Adsorption Evaluations of Shale Gas in Nanometer Pores Based on Molecular Simulation Method

Authors: SUN Renyuan[1]; SUN Ying[2]; TANG Guiyun[2]; GONG Dajian[3]; CAO Haipeng[2]

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

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

[3] *Tongren Zhongneng Natural Gas Company*

Corresponding Authors: sunrenyuan@126.com, 2548147588@qq.com, 407709436@qq.com

Shale gas is one of the unconventional natural gases with huge reserves. The adsorption property is very important for shale gas reserve evaluation and development. By using the molecular simulation method, the shale nanopores model was built and the effects of pressure, temperature and pore size on shale gas adsorption was studied. The simulation results show that, due to the adsorption effect, the average density of methane in shale nanopores is greater than the bulk density of methane at the same conditions. The methane density in the 2nm organic pore is 170 kg/m3 at 10MPa and 303k, while the bulk density is only 74 kg/m3. The difference between the two kind density increases and then decreases with the pressure increasing. The stronger adsorption ability of the media is, the greater the difference between two kind of density. The distribution of methane in nanopores is non-uniform. There is an adsorption layer at pore surface, and the adsorbed layer has a certain thickness and density.
Key words: shale gas, molecular simulation, adsorption, nanometer pore

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How to take into account of clay content in computing elastic moduli of arenites from micro-tomographic images

Authors: Jiabin Liang[1]; Stanislav Glubokovskikh[1]; Boris Gurevich[2]; Maxim Lebedev[1]; Stephanie Vialle[1]; Alexey Yurikov[1]

[1] *Curtin University*

[2] *Curtin University, Australia*

Corresponding Authors: jiabin.liang@postgrad.curtin.edu.au, alexey.yurikov@postgrad.curtin.edu.au, m.lebedev@exchange.curtin.edu.au, stanislav.glubokovskikh@curtin.edu.au, stephanie.vialle@curtin.edu.au, b.gurevich@curtin.edu.au

Derivation of rock physics models for elastic moduli estimation often relies on either simplified models of rock microstructure or empirical relationships established for a particular laboratory data set. Ideally, one would need to calibrate the abstract model parameters to available petrophysical and petrographical (micro-CT images, thin sections, etc.) data. However, elastic properties obtained by numerical simulations for micro-CT images of rock microstructure are considerably higher than those inferred from laboratory measured ultrasonic velocities. Imperfect image segmentation algorithms and image resolution may contribute to this systematic bias. Here, we propose a digital rock physics workflow that provides a robust calibration for velocity-porosity relationships in sandstones with dispersed clay. To this end, we analyse a set of images of Bentheimer sandstone samples accompanied by stress-depended ultrasonic measurements. The results are also compared with the measurements on sandstones by Han et al. (1986).

Quartz is the main constituent of Bentheimer sandstone, with small fraction of feldspar and clay minerals (mainly kaolinite). Bulk and shear modulus of quartz are relatively well defined: bulk modulus K = 37GPa and shear modulus G = 44GPa. Experimental measurements of kaolinite moduli are challenging, with the most convincing experiment (Vanorio et al., 2003) reporting bulk modulus K = 12GPa and shear modulus G = 6GPa. With such contrast, it is important to accurately map clay minerals in the solid material.

Standard segmentation algorithms provide no robust solution to this problem. X-ray absorption for clay particles is similar to that for quartz, they cannot be distinguished by a simple threshold. Here, we propose a new segmentation workflow that relies on both pixel intensity and morphology of clay particles. The main steps are:
• Median filter suppresses random noise and blurs the images;
• Intensity of the clay regions decreases due to presence of micro pores;
• Three-phase Otsu algorithm segments clay together with grain boundary artefacts as a separate phase;
• To remove the grain boundaries from the clay phase, we apply the opening algorithm, which is a sequential erosion and dilation operations, that eventually removes the thin shell-like artefacts;
• Finally, the clay region is used as a mask for the binary segmented image.

This workflow results in a reasonably accurate distribution of mineral phases.

Then, with the moduli computed for scans with different resolution we fit a linear relationship to extrapolate our estimates to the infinite resolution. Our calculation clearly shows that imperfect image segmentation algorithms and image resolution may be considered as the main reasons for the systematic bias between computed and measured moduli. Through the above adjustment, our digital rock physics workflow not only provides a robust calibration for modulus-porosity relationship, but also the modulus-clay relationship for sandstone with dispersed clay.

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A physics based model of gas flow in shales predicts enhanced gas production

Author: Syed Haider[1]

Co-author: TADEUSZ PATZEK [2]

[1] *King Abdullah University of Science and Technology*

[2] *KAUST*

Corresponding Authors: tadeusz.patzek@kaust.edu.sa, syed.haider@kaust.edu.sa

Over the years, most researchers explained enhancements of gas production from shales by invoking slip flow in the nanopores at high Knudsen number, Kn. However, molecular gas dynamics simulations, experimental results in carbon nanotubes, and the calculated Klinkenberg and Brown's slippage factors discredit gas slip at high subsurface pressures (P>3000 psi) and with rough pore surfaces. We propose a model of flow of the high-pressure shale gas, and explain the increased permeability in mudrocks without slip flow and Knudsen diffusion. We predict enhanced gas flow at the outlet of a single micropore, caused by an additional gas influx from the numerous nanopores connected to that micropore. We then extend the single micropore model to a network of micropores, each fed by many nanopores. This network idealizes a microfracture network in contact with organic matrix in a mudrock. The overall permeability increase depends on the nanopore radii, flow rate in the microcapillaries, and the persistence of pressure difference between the nanopores and microcapillaries. A no-flow-reversal condition for the micropore network imposes limits on the nanopore radii and

pressure differentials along the nanopores. We introduce a physical quantity, the microscale source term, s to study numerically the interactions between microfractures and nanopores.

As the average radius of the nanopores feeding the micropore network increases, the ratio of the volumetric flow rates in the micropores, Q_{out}/Q_{in}, increases faster, because the additional gas influx depends on 4th power of the nanopore radius. An increase of the flow rate into a micropore network reduces the effect of the nanopore influx in the system. Q_{out}/Q_{in} is also highly sensitive to the difference between the pressure in the kerogen and that in the micropores. Isolated nanopores in the organic matrix can feed a micropore for only a few milliseconds, demonstrating that the kerogen matrix has a well-connected nanopore network. A small value of the microscale source term, s, gives additional numerical justification for the concept. The effect of the smallest nanopores with the radii < 1nm on the gas storage capacity is highlighted. A mere 5% of such nanopores can maintain a long tail of slow production rate from the mudrock reservoirs.

Our analytical solution captures the experimentally observed enhanced flow rate in mudrocks. It presents a numerical justification for a well-connected nanopore network in the organic matrix, and the impact of the smallest nanopores on the long-term production rate from a horizontal well.

Result Figure for the abstract

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Automatic three-phase segmentation of 3D micro-CT image using deep learning.

Author: Johan Phan[1]

Co-authors: Leo Ruspini [2]; Paal Eric Oeren [3]; Frank Lindseth [4]

[1] *NTNU/Petricore Norway*

[2] *Petricore Norway*

[3] *Petricore*

[4] *NTNU*

Corresponding Authors: leonardo.ruspini@petricore.com, frankl@ntnu.no, paal.eric.oeren@petricore.com, johan.phan@petricore.com

Accurate segmentation of 3D micro-CT images is a crucial process in almost every digital rock workflow. This process is not trivial since micro-CT images have a wide range of artifacts that complicate accurate segmentation. Current segmentation techniques and algorithms are often time-consuming, sensitive to noise and image artifacts, and require skilled people. Deep learning-based 3D segmentation approaches have gained a rapid surge of interest recently in many fields, most notably in

medicine, due to their robustness, high accuracy, self-learning capability, and generalization ability.

In this work, we have built a deep learning model for 3 phase segmentation of micro-CT rock images using a combination of different state of the art methods such as U-net architecture 1, deep supervision [2], hypercolumns [3] and pre-trained SE ResNext encoder [4]. We trained our model on sample images from different CT scanners, where the segmentation target is segmented by us. In order to increase the generalization capability and make our model more robust to noise and artifact, we heavily augmented the training data by using various types of noise and image transformation/distortion.

For validation, we used the ASTRA toolbox [5] to create a synthetic dataset generated from reconstructing the projection of known segmentation images. We measured the sensitivity to noise of the segmentation tool by adding Gaussian noise, beam hardening, and ring artifacts to the synthetic images. Furthermore, we compared the segmentations produced by our tool to those generated by five different experts on three untrained samples: Berea sandstone, Bentheimer sandstone, and a carbonate. We compared the segmentation results in terms of the voxels by voxels differences, phase connectivity, and distribution of phases. By further visual inspection, our tool has successfully demonstrated its robustness to artifacts compared to the segmentation from the experts.

Finally, we have extended our work to make the tool capable of generating higher-resolution segmentation outputs from lower-resolution inputs. In this step, our segmentation tool was able to give high voxel-wise prediction similarity on images that were down-sampled up to 5 times compared to the original.

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Laser-Induced Fluorescence (LIF) study of solute transport in 3D-printed fractured porous media

Author: Mehrdad Ahkami[1]

Co-authors: Xiang-Zhao Kong [1]; Martin O. Saar [1]

[1] *Geothermal Energy and Geofluids Group, ETH Zurich*

Corresponding Authors: saarm@ethz.ch, xkong@ethz.ch, mahkami@ethz.ch

The transport of mass (i.e. solute) plays an important role in various engineering/natural reservoir applications, such as geological carbon dioxide sequestration, migration of contaminants in hydrogeology, and enhanced oil recovery. Natural reservoirs often contain fractures with much higher

permeability than the host rock matrix. These highly permeable fractures are conduits for fast advective transfer of solute, whereas the low-permeability rock matrices could serve as solute retention. Therefore, a thorough understanding of solute transport processes in fractured porous media is of crucial importance for improvements of efficiency of subsurface reservoir applications.

Following our previously-published Particle Image Velocimetry (PIV) measurements (Ahkami et al. 2019), here, we present a laser-induced fluorescence (LIF) study on solute transport in a 3D-printed fractured porous medium. This 3D-printed medium consists of distinct regions with different functionalities to study the effect of these regions on solute transport. Parallel to the flow direction, the medium is equally divided into two porous medium matrices, i.e., a high- and a low-permeability matrix, each with one dead-end fracture and one flow-through fracture. During the LIF experiments, the 3D-printed medium is flooded with water, consisting of Rhodamine-110 tracer, with a diffusion coefficient of 4.3×10^(-10) [m2/s]. The tracer is excited using a green continuous-wave laser with a wavelength of 532 nm. The transport is imaged using a monochrome, 50 MP (6004×5291 pixels) CMOS camera, which is set perpendicularly to the 3D-printed medium and in-line with the laser light.

Using the above image analysis techniques, we delineate the transport of the tracer within the described fractured porous medium. The analyses delineate the role of each region during the tracer transport. Our observations indicate that tracer is being transported to the outlet initially through the flow-through fractures, then the dead-end fractures, and finally the porous matrices. The experimental observations are further quantitatively interpreted using moment analyses, and compared to our lattice-Boltzmann numerical simulations. The spreading extent of tracer into the porous matrices is found to strongly depend on the flooding rate.

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Quantitative Measurement of Supercritical CO2-Water Immiscible Displacement in the Micromodel under Drainage Conditions

Authors: Changzhong Zhao[None]; Yi Zhang[None]; Baokun Zhao[None]; Yongchen Song[None]

Corresponding Authors: zhangyi80@dlut.edu.cn, songyc@dlut.edu.cn, stickzhong@mail.dlut.edu.cn, zhaobaok@mail.dlut.edu.cn

Carbon dioxide sequestration into saline reservoirs is considered as one of the most effective way to mitigate the effect of greenhouse gas. Injection into saline aquifers of supercritical CO2 will lead to fingering and complex displacement patterns, which strongly affects the behavior of CO2 in saline reservoirs. The displacement efficiency and storage safety are two key parameters to evaluate this behavior as for CO2 sequestration. However, the effects of pore-scale characteristics have not been understood well. Therein, supercritical CO2-water immiscible displacement is measured in this study using visualization technology under drainage conditions. An inverted fluorescent microscope and an SCOMS camera are used to record the drainage process. At the same time, fluorescent tracer particles are added into the water to distinguish different phases and work out the velocity field as the micro-PIV. Then serial image analysis is done with the image processing software such as Image J and Photoshop CS6. Therefore, saturations of CO2 during the displacement process and at the quasi-steady state after the drainage, distributions of CO2 and water, velocity field of water, and wettability variation are all calculated under different displacement patterns. From experimental data, it is shown that CO2 saturations and distributions change when displacement patterns change due to different dominant forces and regimes. Haines Jump can be found through the velocity field, which is used to explain the above phenomenon. Meanwhile wettability variation and distributions

are also used for explanation of displacement efficiency. Finally the storage safety is analyzed by different existing forms of wetting phase that can be observed directly through pictures.

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Capturing Dynamic Behavior of Propped and Unpropped Fractures during Flowback and Production of Tight Oil Wells Using a Hybrid Model

Authors: Pin Jia[1]; Linsong Cheng[1]; Ming Ma[1]; Renyi Cao[1]

[1] *China University of Petroleum - Beijing*

Corresponding Authors: lscheng@cup.edu.cn, jiapin1990@163.com, 519507773@qq.com

Hydraulic fracturing, which is realized by injecting fluid and the proppant materials with high pressure to open the formation, has been successfully employed for unconventional oil and gas recovery for decades. During flowback and production, the fracture closure may exhibit with the pressure drop of fracturing fluid dewatering. This paper presented a dynamic fracture model fully coupling flow and geomechanics for flowback, which can comprehensively capture the change of fracture key parameters during the flowback and optimize the strategies of flowback.
This model included two domains: matrix and hydraulic fractures. The matrix flow is simulated by the analytical transient linear flow equation, and dynamically coupled with the fully numerical fracture multiphase flow equation by imposing continuity of pressure and flux. While, the discontinuous displacement method (DDM) is adopted to calculate fractures aperture, and coupled with flow equations by updating dynamic parameters of fractures. Then, the pressure and saturation of each phase in the flow model, along with the normal and shear displacement on the fracture surface are calculated by solving flow equations and geomechanics equations through iterative coupling approach.
The new flow-geomechanics coupled model is validated by comparing with a fully coupled stress-porosity pressure numerical simulation model (Abaqus). The results from the planar fracture case show that fracture closure first occurs at the fracture tip and then gradually moves along the fracture to the fracture heel and then to the wellbore. Flow regime analysis demonstrates that there are five flow periods during flowback and early-time production. These findings are same with that of the previous flowback model without consideration of fracture closure, but the durations of water first linear flow and water first boundary-dominated flow in the fracture become shorter and the hydrocarbon breakthrough occurs later due to the decreasing of effective fracture space. The behavior of a complex fracture network is also be investigated by the new coupling model. With comparison of previous flowback model, the pressure drop around the reactive fracture which is far from the hydraulic fracture is negligible considering fracture closure. Lastly, the fractures key parameters, including the fracture permeability and fracture length after flowback are interpreted by matching real field flowback data.
The new model fully couples multi-phase flow in the fracture and stress which considering the deformation of the fractures. The distribution of the proppant can be set non-uniform and the roughness of fracture is considered. Besides, the fractures key parameters after flowback can be more accurately interpreted by matching flowback data.

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An investigation of the Effect of Gravity on Foam in Model Fractures

Author: Kai Li[1]

Co-authors: William Rossen [1]; Karl-Heinz Wolf [1]

[1] *Delft University of Technology*

Corresponding Authors: k.h.a.a.wolf@tudelft.nl, k.li-2@tudelft.nl, w.r.rossen@tudelft.nl

Gas-injection EOR processes have poor sweep efficiency due to conformance problems including channelling, gravity override and fingering. In naturally fractured reservoirs, sweep efficiency is further jeopardized, because gas breaks through fractures first, leaving most oil behind in the matrix. Strong foam can be created in fractures1[2], thus diverting the flow of gas into matrix and hence increasing the oil recovery[3]. In the field, natural fractures are usually vertically oriented, because the least principal stress is in horizontal direction in most formations. Foam performance in fractured reservoirs is affected not only by fracture roughness, aperture, etc., but also by gravity. In this study, we investigate how gravity affects foam in fractures. To this end, we have conducted several sets of foam-scan experiments (i.e., a set of constant-total-velocity experiments, each with a different gas fractional flow) on three glass model fractures (model A, model B and model C) with hydraulic aperture of 78, 99 and 128 μm respectively.
The models have the same dimensions of 1 m x 0.15 m (L x W) and the same fracture roughness pattern. The transparency of glass models allows a direct investigation of foam texture inside the fracture using a high-speed camera. All experiments have been carried out at 20℃ and 1 atm. Nitrogen is the gas phase, and surfactant solution is 1 wt % AOS C14-16.
Experiments were carried out on all three models by placing the model either horizontally or on its side. Stable foam was created and reached local equilibrium in all horizontal-flow experiments: the rate of foam lamella creation was equal to the rate of destruction. The roughened fracture surface provided sufficient generation sites to re-create foam bubbles in sections further from the entry, hence maintaining a stable foam.
In the sideways flow experiment, the effect of gravity on foam stability was not significant when fracture aperture was small (model A). As hydraulic aperture increased (model B and model C), the effect of gravity was more pronounced. Drier foam propagated along the top part of the fractures and wetter foam along the bottom. Gas saturation was 18% greater at the top than the bottom for model B, and 27% for model C. Foam was still stable during the sideways flow experiments in model B. However, foam breakage alternated with re-generation near the top in model C.
We conclude that the application of foam in vertical natural fractures (meters tall and tens of meter long) with an aperture of hundreds of microns is problematic. The gravity segregation of phases for the foam in our experiments would disable its capacity to divert gas flow from a tall fracture like our model into the matrix. As a result, there would be a gas-rich regime at the top of the fracture and a liquid-rich regime at the bottom. The regimes segregate more as the aperture increases.

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Level set based automatic in-situ contact angle measurement

Author: Yingfang Zhou[1]

Co-author: Jianhui Yang [2]

[1] *University of Aberdeen*

[2] *GRC, TOTAL*

Corresponding Authors: jianhui.yang@total.com, yingfang.zhou@abdn.ac.uk

Contact angle is one of the key petrophysical properties that control multiphase flow in porous media as it determines the pore scale fluid configurations and displacement mechanisms (Blunt, et al., 2013; Zhou, et al., 2014). Contact angle defined at the three-phase (one solid and two immiscible fluids) contact line is normally measured outside a porous medium using either sessile drop method or pendent droplet method on a smooth solid/rock surface. This ignores complexities such as pore surface roughness, pore size, non-wetting droplet size and mineral heterogeneities. The use of advanced imaging technologies, such as micro-CT, have made it possible to image the fluid distribution inside the pore space and thus provide us an alternative approach to estimate contact angle directly (Andrew, et al. 2014); this approach allows us to measure in situ contact angles for which several automatic approaches have been proposed (for instance, Klise, et al., 2016; Scanziani, et al., 2017; AlRatrout, et al., 2017).

The most recent automatic approach (AlRatrout, et al., 2017) was implemented in the OpenFoam platform and requires parameter tuning to produce smooth surface. In this work, we developed a purely mathematically defined level set based method to calculate the effective contact angle directly from imaged fluid configurations in pore space; this method includes three steps to estimate contact angle based on imaged pore scale fluid configurations. First, reinitialize and build up level set function for both solid phase and non-wetting phase; second calculate normal vectors for both fluid-fluid and fluid-solid interface based on the two pre-determined level set functions; and then estimate contact angle as the dot product of vectors.

We first validated our newly proposed method for the fluid configurations that simulated at a 2D cross section using the semi-analytical method (Zhou, et al., 2014) and then we also tested the algorithm on a synthetic spherical oil droplet residing on a titled flat solid surface where the contact angle is analytical defined. This newly proposed method was then used to measure the in-situ contact angle of a droplet directly imaged by micro-CT technical and the results are compared with the manually (Andrew, et al. 2014) and other available automatic measured (Scanziani, et al., 2017) contact angle. The measured in-situ contact angle distributions for these high-resolution droplets are comparable with that measured from other approaches, what's more, this approach is well mathematically defined with equations, it doesn't require any other complicated tuning procedure for surface smoothing.

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Experimental study of corner flow using 2.5-D microfluidic porous media

Authors: Guanju Wei[1]; Ran Hu[1]; Zhen Liao[1]; Yifeng Chen[1]

[1] *Wuhan University*

Corresponding Authors: zyliao@whu.edu.cn, weiguanju@163.com, csyfchen@whu.edu.cn, whuran@whu.edu.cn

Corner flow is an important phenomenon during the fluid-fluid displacement in porous media and has been studied extensively. Previous studies focused on the experiments using 2-D micromodel or angular capillaries, these micromodel lacked the connectivity between grains and this connection should facilitate corner flow. Here we study the corner flow phenomenon on favorable immiscible fluid-fluid displacement by means of microscope in 2.5-D microfluidic. Strong imbibition experiments of oil displacing air were conducted at eight flow rates (capillary number ranging from 6.3×10-4 to 2.5×10-6). The whole experimental processes were recorded using a microscope with a CCD camera. As the flow rate decreases, we observe that the displacement front becomes unstable and corner flow happens more easily. Compared with the 2-D microfluidic experiments, the displacement front is highly unstable where corner flow dramatic happens, thus a large volume of the defending phase is trapped in the micromodel.In order to gain more information about the fluid-fluid displacement in 3-D, we calculate the displacement efficiency based on the Beer-Lambert absorption law. The results show that there is a sharp change in the displacement efficiency at the flow rate of 1.25 ul/min(Ca=3.15×10-4) and the displacement efficiency decreases with the decrease of the flow rate, which means that corner flow is sensitive to the flow rate in favorable immiscible displacement. Our work is the first time to observe the corner flow phenomenon and reveal the rule of favorable immiscible displacement in 2.5-D microfluidic by means of microscope, improving our understanding of multiphase flow during strong imbibition conditions where corner flow occurs.

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Small Angle Neutron Scattering to determine the Interplay between Fluids and Pores in Mudrocks

Authors: Amirsaman Rezaeyan[1]; Timo Seemann[2]; Pieter Bertier[3]; Vitaliy Pipich[4]; Lester Barnsley[4]; Andreas Busch[1]

[1] *Heriot-Watt University*

[2] *RWTH Aachen University*

[3] *Dynchem Scientific Instrument*

[4] *Forschungszentrum Jülich GmbH*

Corresponding Authors: a.busch@hw.ac.uk, ar104@hw.ac.uk

Mudrocks feature geological and geotechnical applications such as unconventional resources of fossil fuels, source rocks as well as caprocks for conventional hydrocarbon accumulations or above H2/CO2 storage sites, as well as host rocks for radioactive waste disposal. The exploitation of mudrocks requires characterisation of pore structure over the entire pore size range. Small angle neutron scattering (SANS) was used to quantify both accessible and inaccessible pores with sizes ranging between ~1nm and ~20µm, which is relevant for mudrocks. SANS experiments were carried out on various mudrock samples to understand porosity as well as investigate the effect of depositional and post-depositional controls on the pore architecture of mudrocks at different scales. The distribution

of pore sizes can be used to determine dominant flow regimes, such as Darcy, slip or diffusional flow. Injection of supercritical fluids (CO2 and CD4) into the pore space of mudrocks at high pressures and temperatures (up to 46 MPa, 50°C), the phase behaviour depending on pore size was investigated with subsequent neutron scattering. Results obtained from supercritical fluid sorption within SANS experiments demonstrated the formation of an adsorbed phase with the density and volume fraction varying with pressure, temperature and pore size, affecting sorption mechanism, gas storage and production. Analysing pore size distribution, SSA and porosity in relation to pore orientation and fluid flow regime provides important input to pore network and Lattice-Boltzman models to improve our understanding of fluid transport and sorption mechanism in mudrocks.

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Coupling between the dynamic capillary pressure and deformation in porous materials

Author: YULIANG ZOU[1]

Co-authors: Frédéric GRONDIN [1]; Mazen SAAD [1]

[1] *Ecole Centrale de Nantes*

Corresponding Authors: mazen.saad@ec-nantes.fr, frederic.grondin@ec-nantes.fr, yuliang.zou@ec-nantes.fr

In the case of a fast drying process, water movements result in a rapid change in capillary pressure. As a negative tension, capillary pressure is the main cause of shrinkage during drying in porous media [1,2]. These deformations are often the cause of the occurrence of micro-cracks and must be mastered [3]. To predict these risks, experimental procedures and highly sophisticated models have been developed by researchers around the world. Probabilistic laws are defined regarding experiments so as to predict the risk, and models are proposed to approach real phenomena based on physical relationships. However, differences are observed between numerical results and experimental results, owning to a phenomenon little known: the dynamic effects on the capillary pressure (difference between the pressure of two fluids) when the saturation in porous media experiences a fast change [4]. Under dynamic condition, the viscous forces are non-negligible and needs additional pressure gradient to overcome. The pressure difference between gas mixture and liquid water may deviate from the initial static capillary pressure [5]. Until now the models used to predict the deformation of most porous media are based on the quasi-static behaviour laws, and dynamic effects are completely neglected.
In this paper, a new coupling model between solid deformation and fast fluid transport is proposed. An innovative mathematical dynamic coupling model is deduced from the combination of dynamic

capillary pressure law, Richards'equation and principle of effective stress. Then this dynamic coupling model is compared with static coupling model to observe its influence on mechanical deformation and capillary pressure evolution. A 2-D plane strain simulation is carried out to verify the impact of this innovative coupling model through finite element software COMSOL Multiphysics. Simulation results demonstrate that dynamic effects on capillary pressure not only accelerate the decrease of saturation, but also enlarge the deformation of porous media. Furthermore, dynamic effects significantly increase the possibility of cracks occurrence, especially at the area close to surface of porous materials and during the stage that boundary conditions experience rapid variation.

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Foam Trapping and Foam Mobility in a Model Fracture

Author: Kai Li[1]

Co-authors: William Rossen [1]; Karl-Heinz Wolf [1]

[1] *Delft University of Technology*

Corresponding Authors: k.h.a.a.wolf@tudelft.nl, w.r.rossen@tudelft.nl, k.li-2@tudelft.nl

Gas injection often suffers from the poor sweep efficiency because of conformance problems, including gravity override, viscous fingering and channelling, since gas has a lighter density and a lower viscosity compared to in-situ fluids. Foam, by encapsulating the gas into separate bubbles in surfactant-coated liquid thin films (lamellae), can effectively address the conformance problems and hence improve the sweep.
Strong foam can reduce gas mobility by a factor of hundreds, by trapping gas and reducing its relative permeability in situ1. To efficiently improve the sweep, foam needs to propagate and maintain its strength at locations further away from the injection well. Foam trapping and propagation are highly dependent on porous media geometry, injection rate, foam quality, etc.
Microfluidic system, a medium integrating flow channels of manipulated structures on the order of tens to hundreds of microns, have been increasingly attractive to oil and gas, chemical and pharmaceutical research[2]. Microfluidics are also becoming one of the most stimulating research fields in foam EOR, because it provides the opportunities to visualize foam behaviour directly, such as foam generation, propagation and foam coarsening[3], etc.
We employ a model similar to microfluidics, directly applicable to flow in geological fractures. The 1-meter-long model represents a fracture channel with one roughened and one smooth wall. It has a width of 15 centimeters and a hydraulic aperture of 128 μm. The model is made of glass plates, therefore enabling direct investigation of foam behaviour through the channel using a high-speed camera. Since roughened glass is available with a range of roughness scales[4], one can relate foam behaviour to the roughness pattern in the channel.
We conduct a series of foam experiments in the model. Local equilibrium of foam (i.e. the rate of bubble generation equals to that of bubble destruction) is reached within our long model. We study the dynamics of gas trapping at different velocities and gas fractional flows.

We observe that velocity affects the fraction of gas which is trapped in the model at low foam qualities. Gas trapping decreases and foam mobility increases as superficial velocity increases. This contributes to shear-thinning mobility of the foam. At high foam qualities, the relation between trapped gas and foam mobility is weaker. Gas trapping is insignificant and has little effect on foam mobility. When gas fractional flow increases at high foam qualities, flow alternates between slugs of gas and foam.

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Ferrofluid-Enhanced Mobilization of Trapped Oil: Microfluidic And Numerical Investigation

Authors: Ningyu Wang[1]; Yifei Liu[2]; Matthew Balhoff[3]; Masa Prodanovic[1]

[1] *The University of Texas at Austin*

[2] *China University of Petroleum (East China); The University of Texas at Austin*

[3] *University of Texas at Austin*

Corresponding Authors: wang.ningyu.ut@gmail.com, masha@utexas.edu, balhoff@mail.utexas.edu, lyfupc@163.com

Ferrofluids are stable dispersions of paramagnetic nanoparticles (<100nm) in a liquid carrier that are magnetically controllable. As their surface can be functionalized to selectively attach to different surfaces, they have a range of applications from localized heating in biomedical applications to magnetic field control of valves in microelectromechanical devices. They can also be designed to flow through the rock pore spaces without retention, and we here investigate the use of ferrofluids to mobilize trapped oil using microfluidic experiments and computational fluid dynamics.
Single-channel glass micromodels with varying depth (a.k.a. 2.5D) and pore/throat sizes in 10-100 micron range were fabricated using a standard lithography procedure (Xu et al, 2017). The micromodels were initially saturated with brine and then saturated with crude oil or decane. Ferrofluid was subsequently injected at 0.1 μL/h to displace the oil until steady state residual oil saturation was achieved. All changes were monitored under microscope and recorded using a high-speed camera. A magnetic field was then applied to study the effects of ferrofluid on deformation and mobilization of trapped oil resulting in oil saturation reduction. We built a finite element method numerical model that coupled the Navier-Stokes equations for flow and Maxwell equations for the magnetic field in order to explain mechanisms for observed residual oil reduction.
Oil droplet deformation (from spheres to ellipsoids), dynamic break-up into smaller droplets, and subsequent residual oil saturation reduction was observed in micromodels with the presence of magnetic field, but not without one. During ferrofluid flooding, the oil saturation within the observation area of micromodel reduced from 27.0% to 4%. Numerical simulation results showed that the deformation of the oil droplet was caused by a non-uniform pressure field around the oil droplet induced by the magnetic field. The magnetic pressures depend locally on the magnetic field intensity and the direction of the field. Ferrofluid interfaces represent magnetic permeability discontinuities, and as ferrofluid-oil interface dynamically changes, it causes disturbances in the spatial distribution of the field and resulting magnetic pressures.
We show experimentally how ferrofluid, in the presence of a magnetic field, works towards decreasing residual oil saturation and explain underlying mechanisms. The magnetization of ferrofluids

incurs stress on trapped oil interfaces that help displace oil droplets. A synergy of methods such as surfactant injection and ferrofluids in a magnetic field has a potential to reduce trapped oil saturation near the wellbore.

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Validating pore-scale modeling of fluid flow and mass transport in multi-scale porous media with microporosity

Authors: Bin Wang[1]; Karsten Thompson[None]; Richard Hughes[1]; Lin Mu[2]

[1] *Louisiana State University*

[2] *University of Georgia*

Corresponding Authors: linmu@uga.edu, rghughes@lsu.edu, karsten@lsu.edu, binwang.0213@gmail.com

Direct numerical simulation (DNS) of pore-scale fluid flow and mass transport in micro-CT images of rock samples is becoming a standard tool in digital rock analysis. When the micro-CT images of heterogeneous rocks contain unresolved microporosity, an accurate prediction of bulk permeability and solute transport using DNS remains a challenge [1, 2]. Recently, a multi-scale DNS using the Brinkman equation was applied to address this issue. where the stokes equation and Darcy equation are adopted to resolved macroporosity and unresolved microporosity, respectively [2, 3]. For the multi-scale DNS, an accurate porosity and permeability estimation of the unresolved microporosity can play an important role in predicting bulk permeability [2]. However, it is still a challenge to estimate the porosity and permeability of microporosity from the low-resolution micro-CT image and to incorporate other upscaled parameters that enable modeling of solute or particle transport and reaction in the microporous regions.

In this work, we present a validation of multi-scale DNS in a semi-synthetic porous media by embedding geometrically-based microstructure into micro-porous regions of a micro-CT image. A Berea sandstone micro-CT image [4] with 14% macroporosity and 3% microporosity is segmented into three phases, the non-porous solid, the macroporosity and the microporosity. The model of the porous region (including both macroporosity and microporosity) is thus obtained from micro-CT images, but with a range of geometric packings embedded into the microporous regions to represent their hypothetical structure. With the fully resolved microporosity, the flow field is solved using the Stokes equation on a multiscale mesh, the results of which are compared to the multi-scale Brinkman equation with upscaled permeability from the geometric packings. Finally, comparisons between simulations using the multi-scale Brinkman equation and the Stokes equation are made with regard to the estimated bulk permeability values, the pore velocity flow field, the breakthrough curve and the solute concentration field for both solutions.

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Numerical Simulation of Fault Slip in Shale Gas Reservoirs Based on Discrete Fracture Network Model

Authors: Hao Liu[1]; Zhaoqin Huang[1]; Qinghua Lei[2]

[1] *Center of multiphase flow in porous media, China university of Petroleum (East China)*

[2] *Department of Earth Sciences, ETH Zürich*

Corresponding Author: 765758668@qq.com

Abstract:
During the hydraulic fracturing process, fluid will be pumped into the natural fractures due to the development of fracture network in the shale gas reservoir. As a result, the pressure within the fractures will increase, which could activate the natural fractures and lead to the faults slipping. In this work, a fully coupled two-phase hydro-mechanical model is established based on the discrete fracture network (DFN) model for analyzing the fractures'shear slip. The adsorption and desorption effects of shale gas in the formation as well as the pressure-sensitive effects are considered. The rock properties of the matrix and fractures such as porosity and permeability will change during the hydro-mechanical coupling process. The beddings and fractures are characterized by a nonlinear joint model, which considers the compression-induced closure and shear-induced dilation. The behavior of natural fractures in response to various stress conditions illustrates a range of realistic behavior including closure, opening, shearing and dilation. The method is validated by a test of conceptual model. And then, the effects of different parameters on the fault slip including different fault location, injection rates and fluid properties are analyzed.

Key Words:
Discrete fracture network model, rock deformation, shear dilation, two-phase flow, hydro-mechanical coupling

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The Implementation of Ensemble Kalman Filter in Automatic History Matching for a Marine Reservoir and a Fluvial Reservoir

Author: Zelong Wang[1]

[1] *PetroChina*

Corresponding Author: zelongwang10@126.com

In reservoir management, using all the observed data to update the reservoir models is a fatal part to predict the parameters changing and future production. Ensemble Kalman Filter (EnKF) provides a practical way to continuously update the petroleum reservoir models, at the same time; it ensures the recent measurements are consistent with the initial values.
In this paper, we mathematically demonstrated Ensemble Kalman Filter method; discussed its advantages over standard Kalman Filter and Extended Kalman Filter (EKF) in reservoir monitoring, and its limitations. Two case studies will be conducted using the EnKF to update static parameter permeability, and dynamic parameters such as pressure, water cut. One is using the EnKF for updating marine reservoir models, the other one is for updating fluvial reservoir models. A comparison of the results from the two case studies is made, and some suggested adjustments of the EnKF for its application in fluvial reservoirs are presented.

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Influence of reservoir heterogeneity on fracture propagation of true triaxial hydraulic fracturing

Author: Jin Wang[1]

Co-authors: Jianwei Feng [1]; Rongtao Jiang [2]; Wenqing Tang ; Ping Wang [2]

[1] *China University of Petroleum*

[2] *China University Of Petroleum*

Corresponding Authors: 478684961@qq.com, jiang_rtcs@163.com, 1404195190@qq.com, 337638979@qq.com, 846396194@qq.com

Abstract: the effect of true triaxial hydraulic fracturing system on the propagation of heterogeneous fractures in reservoirs is studied. Because the reservoir heterogeneity of delta front is obvious, and it is also a good reservoir space for oil, water and other fluids, the lithologic combination model of Putaohua formation reservoir in delta front of Songliao basin is selected as the template. Three kinds of artificial cores with interbedding of silty mudstone, argillaceous siltstone and siltstone are designed according to the development law of interbedding of sandstone and mudstone. The true triaxial hydraulic fracture simulation experiment is carried out first, and then the core is simulated by ANSYS software. Combined with two kinds of experimental results, it is shown that when the reservoir has pre-existing fractures, the fracture mode of rock samples mainly consists of three modes: sliding failure along the early pre-existing fractures, new fractures generated along the stress change of rock samples, and composite failure of new fractures and primary fractures. When the lithology has vertical stratification and horizontal stratification, the fracture position of the rock sample is generally closely related to the perforation position and the number of perforations. However, if the core permeability is high, the fracture expansion space will become larger, thus improving the core fracture ductility. Generally, the fracture will break from the elastic layer with relatively low permeability. The linear density of fracture is the highest but the smallest in silty mudstone, and the largest in argillaceous siltstone。
Key words: true triaxial hydraulic fracturing ;reservoir heterogeneity ； Songliao basin

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Stress Field Change of Multi well and Multi period Fracturing and its Influence on Reservoir Development

Author: Rongtao Jiang[1]

Co-authors: Jianwei Feng [2]; Jin Wang [2]

[1] *China University Of Petroleum*

[2] *China University of Petroleum*

Corresponding Authors: 337638979@qq.com, 478684961@qq.com, jiang_rtcs@163.com

Abstract:Tight reservoirs are becoming more and more important in the development of oil and gas in the world at present, Hydraulic fracture of.reservoir has become one of the main means to solve the problem of low porosity and low permeability in unconventional reservoirs. The formation of the hydraulic fracture is controlled by the stress field, which always extends along the direction of the maximum principal stress. The change of the stress field in the process of hydraulic fracturing will directly affect the expansion and development of the reservoir fracture.In this paper,researchs are studied that multi-well simultaneous hydraulic fracturing and multi-stage hydraulic fracturing based on the two-dimensional flat model of XFEM.The simulation results show that the stress intensity at the fracture tip is always the largest, and it is a area that is the most easily fractured in the process of fracturing.The weak part in the same stress field will be preferentially fractured due to the influence of hydrofracture. When there is an angle between the perforation direction and the direction of regional maxmum principal stress, the extension direction of the hydraulic fracture is always consistent with the maximum principal stress direction of the local at any time.The local stress field appears tensile stress near the fracture. At the same time, the local tensile stress field near the fracture will increase the minimum principal stress in the surrounding area, which will cause the dominant direction of one fracture to hinder the expansion of the other;and the early fracture will hinder the expansion of the fracture due to the leakage pressure.
Key words: unconventional reservoir; fracture; stress field

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Oxidative dissolution during spontaneous imbibition in organic-rich shale: implication for the matrix stimulation

Authors: Qiuyang Cheng[1]; Lijun You[1]; Yili Kang[1]; Yang Zhou[1]; Nan Zhang[1]

[1] *SWPU*

Corresponding Authors: cwctkyl@163.com, youlj0379@126.com, cqygm@foxmail.com

Facing large of fracturing fluid retention and exponential reduction of shale gas well production after hydraulic fracturing, converting detrimental fluid retention to beneficial force continuously stimulating the reservoir thereby may be a feasible strategy reducing costs and increasing profits. Outcrop shale fracturing caused by oxidative weathering is important implication for shale matrix stimulation. This work is to investigate the feasibility that the imbibition of oxidative fracturing fluid into shale after hydraulic operations continuously enhances stimulated reservoir volume at micro- and nano-scale. Spontaneous imbibition is regarded as an important mechanism for fracturing fluid retention, we thereby used shale plugs exploring the imbibition behavior of oxidative fluid by contrast of the imbibition behavior of deionized water (DI water); shale cubes (5 × 5 × 5 mm) respectively were exposed into DI water and oxidative fluid revealing the change in structure before and after the treatment by field-emission scanning electron microscopy (FESEM). To reveal the mechanism that oxidative fluid induced the structure changes, two group crushed shale samples (380–830 μm) were exposed to oxidative fluid in a closed container; change in shale components was determined by X-ray diffraction; the gas products and associated pressure enhanced in the container were measured. Experiments show a higher imbibition potential of DI water in artificial fracture samples in the early, corresponding to a "B"shape of imbibed volume vs sqrt time curve; DI water inducing microfractures effectively in the matrix samples resulted in a "J"shape, promoting the imbibition potential; oxidative fluid accelerates the matrix samples fracturing obviously promoting the imbibition potential, and the curves present a "S"shape. SEM imaging shows oxidative fluid not only creates lots of dissolution pores like the effect of acid fluid, and induces much more microfractures than DI water. Dissolution pores seemed to strongly depend on the loss of calcite, dolomite, and pyrite; and the microfractures initiation and propagation attributes to the combined effect of oxidative dissolution, crystallization and enhanced pore pressure. Results indicate that a coordinative effect between spontaneous imbibition and oxidation inducing pores and microfractures can play a role in continuously matrix stimulation after hydraulic fracturing. This study lays a foundation for no flowback of oxidative fracturing fluid improving gas transmission capacity of the matrix to enhance shale gas recovery.

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Equivalent Conductivity Tensor in 3D Anisotropic Heterogeneous Formations

Authors: Qinzhuo Liao[1]; Gang Lei[1]; Dongxiao Zhang[2]; Shirish Patil[1]

[1] *KFUPM*

[2] *SUSTech*

Corresponding Authors: liaoqz@gmail.com, patil@kfupm.edu.sa, zhangdx@sustech.edu.cn, gang.lei@kfupm.edu.sa

Modern geological modeling techniques represent anisotropic heterogeneous formations by high-resolution grids, which can be computationally prohibitive. This motivates the upscaling process that scales-up properties defined at a fine-scale system to equivalent properties defined at a coarse-scale system. In general, analytical methods are very efficient but limited to assumptions and approximations, whereas numerical methods are more robust albeit more time-consuming.

In this work, we develop an analytical method to approximate numerical solutions in a finite difference scheme with periodic boundary conditions. Using perturbation expansion techniques and Fourier analysis, the method generates explicit formulas of tensorial equivalent conductivity considering heterogeneity and anisotropy of 3D space, as well as geometry of gridblocks. It is applicable for various cases with different covariance/variagram models and a wide range of log-conductivity variances, correlation lengths, rotation angles, anisotropy ratios of fine grid conductivity, anisotropy ratios of fine grid size, and the number of fine gridblocks in a coarse gridblock. The coefficients in the analytical method need to be computed only once for any given statistics, which makes the proposed method much more efficient than the numerical method.

We test the method in synthetic examples and benchmark cases with both Gaussian random fields and channelized non-Gaussian fields. The analytical method matches well with the numerical method for the estimation of the conductivity tensor, hydraulic head, and discharge velocity. In addition, we examine the impact of each parameter on the upscaled conductivity, and investigate the sensitivity of the variance and correlation lengths to the coefficients. This approach can also be extended to multiphase flow problems using pseudo-relative permeability functions.

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A SEM Study on the "Smart Water"Assisted Polymer Flooding in Sandstone Reservoirs

Authors: Hongna Ding[1]; Xinjian Tan[1]

Co-authors: Fajun Zhao [1]; Jihong Zhang [1]

[1] *Northeast Petroleum University*

Corresponding Authors: klmytxj@163.com, fajzhao@126.com, hongnading1989@hotmail.com, dqzhjh@126.com

In recent years, "smart water"flooding and its associated techniques such as smart water assisted polymer (SAP) flooding have aroused great interest in petroleum industry. The SAP flooding is supposed to be a promising technology for enhancing the oil recovery of offshore reservoirs, which might lead to equal or even higher oil recovery than the sum recovery of smart water flooding and polymer flooding. The performance of SAP flooding depends largely on the types of smart water and polymer comprising of a certain SAP system, as well as the rock mineralogy, especially considering its effectiveness in altering the rock wettability, mobilizing the capillary trapped oil and improving the sweep efficiency. Up to date, the SAP flooding is little studied in laboratory, which has limited its

application at oilfield. In this study, we intend to fill part of the void by conducting a subscale study with respect to the interactions between sandstone and different SAP systems (which were prepared by formation water and formation like waters) using scanning electron microscope (SEM). The SEM results showed that the polymer molecules primarily adsorbed on clay mineral surfaces rather than quartz surfaces due to the strong cation exchange capability of clay minerals. In the case of formation water, the SAP system existed as large aggregates in micro- and nano-pores, showing an irregular cotton-like morphology on clay surfaces, which can be attributed to the strong cation bridging interactions between the clay mineral and the SAP system. In contrast, the morphology of SAP system on clay surfaces changed to honeycomb-like configuration using iron-depleted formation water or sulfate-enriched formation water, especially when the sulfate concentration in formation water was increased up to 4-6 times, which suggested that the cation bridging interactions were mitigated by these two smart waters. Our results also showed that the calcium- or magnesium-depleted formation water, in which the concentration of calcium ions or magnesium ions was reduced to less than half, had positive effect in reducing the cation bridging interactions, resulting in regulated structures of SAP systems on clay surfaces. The microscopic to nanoscopic observations of SAP-rock interactions in our study are possible to give hints on the promising ingredients of SAP flooding in sandstone reservoirs.

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Pore Structure Analysis for Exhaust Particle Filter Development

Author: Atsushi Tanaka[1]

Co-authors: Naoto Miyoshi [1]; Akemi Sato [1]

[1] *Toyota Motor Corporation*

Corresponding Author: atsushi_tanaka_ag@mail.toyota.co.jp

In response to awareness of environmental protection, development of eco-friendly vehicle is required. Conventional internal combustion engine vehicles are still occupying a majority and it has high demand to reduce exhaust gas emission such as NOx, CO, hydro-carbon (HC) and also particulate matters (PM). To reduce PM emission, suppressing the emission by improvement of engine combustion and applying the gasoline particulate filter (GPF) is required. It is effective to load a certain amount of washcoat on GPF to add three-way purification performance, but it leads the filter pore to be filled with washcoat and increase the pressure drop that affected the engine power. To understand the influence factor of the wall permeability which affected pressure drop, the pore structure with different washcoat loading was analyzed by utilizing mercury porosimetry and micro X-ray CT which enabled 3D model structural analysis. As a result, it was confirmed that the number

of percolation path was decreased significantly by the washcoat loading. In addition, the contribution of the diameter of each percolation path was analyzed by applying the permeability model. It was clarified that the amount of the narrow percolation path had influence on permeability.

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Effect of Oil Polarity on the Time-Scale of Mixing during Low Salinity Waterflooding: A microfluidic Investigation

Authors: Saheb Mohammadi[1]; Hassan Mahani[1]; Shahab Ayatollahi[1]; Vahid.J Niasar[None]

[1] *Sharif University of Technology*

Corresponding Authors: vahid.niasar@manchester.ac.uk, hmahani@sharif.edu

Low salinity water flooding (LSWF) is an enhanced oil recovery (EOR) method which is based on injecting a brine, with manipulated salinity and ionic composition, typically of total salinity less than the in-situ formation water. The efficiency of LSWF is highly influenced by mixing, particularly between the stagnant zones containing high salinity water and the flowing zone containing low salinity, since it impacts directly the kinetics of wettability alteration by low salinity.

This study aims to address the impact of oil polarity and charged rock surfaces on the time-scale of mixing and transport under two-phase flow conditions. Although the role of charged surfaces on delayed transport has been discussed in the published literature, to our knowledge, no experimental work has been reported in the literature to address the role of oil polarity in transport. To do so, we first developed two different glass micromodels with two different pore structures which make different trapped oil geometries and stagnant zones. We then used different types of oils with different polarity including model and crude oils. We investigated the effect of oil polarity on time-scale of mixing by continuous monitoring of selected parts of the micromodel with stagnant saturation. Finally, CFD simulations were performed to reproduce the experimental results and infer the effective diffusion coefficients corresponding to the experimental conditions.

The results show that under a salinity gradient, the time-scale of mixing can be influenced by the electric charge of the oil and rock surfaces in which case the Fickian diffusion model cannot explain the phenomenon anymore. The experimental results indicated that by increasing oil polarity (by adding carboxylic groups), the mixing is slowed down 10-20 times which is postulated to be due to the stronger electrical field induced in the film by oil polar components. The stronger electrical field limits the salt transport rate according to the Nernst-Planck theory. In the case of using crude oil which is highly polar and contains complex types of polar groups such as resins/asphaltenes, the time-scale increase is the largest. The CFD simulation confirms that the effective diffusion coefficient (which can be influenced by oil polarity) is the predominant factor determining the time-scale of mixing. But nevertheless, amongst the other factors such as film thickness/length and the salinity gradient, the film thickness/length has the dominant effect on mixing phenomenon.

This study brings new insights into the minimum required time to replace high salinity water with low salinity water especially in dead-end pores that plays the most important role on the kinetics of wettability alteration and the required amount of low salinity water to be injected to observe the low salinity effect (LSE).

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Micro Perspective of Capillary Force Hysteresis: Theoretical and Experimental Research on the Relationship Between Capillary Pressure and Saturation in Microscale Capillaries

Author: Menggang Wen[1]

Co-author: Yun Li [1]

[1] *School of Chemical Engineering and Technology, Xi'an Jiaotong University*

Corresponding Authors: yunli@mail.xjtu.edu.cn, wenmenggang@stu.xjtu.edu.cn

Capillary pressure curve is a basic characteristic of immiscible two-phase seepage in the oil reservoirs and an important relationship curve for oilfield developments. Many studies have reported the relationship between the capillary pressure and the wetting phase saturation, and found the capillary pressure hysteresis, i.e., the capillary pressures are different at the same saturation during a full imbibition-drainage cycle. At the macroscale, fluids are supposed to coexist in the reservoir porous media with each occupying a fraction of volume. Capillary pressure at the macroscale is considered as a function of the reservoir properties, fluid physical properties, and saturation of the wetting phase. At the microscale, capillary pressure is a property of the fluid interfaces and is not directly determined by the pressure in the fluids juxtaposed on the interface. In this study, with the objective of comprehending the characteristics of capillary pressure hysteresis on the macroscale from the microscale perspective, capillary pressure hysteresis of the quasi-static imbibition-drainage process in a single microscale capillary tube was performed. Based on the Helmholtz free energy analysis of a two-phase isothermal system in a single microscale capillary tube, a partial differential function between the capillary pressure, interface mean curvature, and contact angle was established under the minimum functional constraint. Quasi-static imbibition-drainage experiments were conducted in microscale capillary tubes to verify the partial differential model. The interfaces were tracked and captured with a fixed focus digital microscope (Cewei Guangdian, Beijing) (2x objective lens) with a 1600-MP CMOS (DigiRetina 16). High-contrast two-phase images were observed by the reflected light (top light source on the microscope). All the two-phase images were treated by a grey threshold method to create binary images. Phase interface curves were fitted to obtain the interface mean curvatures and contact angles to calculate capillary pressures. The experimental results were in great agreement with the analytical solution of the model, i.e., capillary pressure exhibited hysteresis during an imbibition-drainage cycle. The results showed that capillary pressure could reverse during contact angle hysteresis. This phenomenon is a manifestation of the liquid wettability reversal caused by contact angle hysteresis. In addition, capillary pressure hysteresis in different saturation ranges was investigated, which exhibited similar characteristics that is observed in the plastic hysteresis and magnetic hysteresis. Furthermore, capillary pressure hysteresis in microscale capillary tubes with variable cross sections was studied. The results showed that the microscale capillary tube sizes and structures exert significant effects on the capillary pressure hysteresis pattern.

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An image recognition method for gas/liquid saturations and investigation of air-liquid threshold displacement pressure with dispersed bubbles in the planar pore network

Author: Menggang Wen[1]

Co-author: Yun Li [1]

[1] *School of Chemical Engineering and Technology, Xi'an Jiaotong University*

Corresponding Authors: wenmenggang@stu.xjtu.edu.cn, yunli@mail.xjtu.edu.cn

Two-phase threshold displacement pressure is the minimum pressure corresponding to the displacing phase forming a through path in the porous media. Threshold pressure is crucial to determine the minimum overpressure required for the reservoir seepage processes, such as in the geological storage of CO2 and enhanced oil and gas recovery. Many experiments have been carried out to study the threshold pressure of single-phase percolation, but related studies on the threshold pressure of two-phase displacement have rarely been reported. In addition, since dispersed bubbles could generate in crude oil under reservoir conditions, the effect of the dispersed bubbles on the two-phase threshold displacement pressure is puzzled. The main purpose of this investigation was to study the threshold pressure of air-liquid displacement with dispersed bubbles. Air-liquid quasi-static visualization displacement experiments were performed in planar pore networks. The planar pore networks were etched on the 1 mm borosilicate glass using wet etching and bonded with 1 mm borosilicate glass at low temperature. In displacement experiments, a pressure transducer (with an accuracy of 0.5%FS) was installed at the pore network inlet to record the displacement pressure in real time within ±50 kPa. The displacement patterns were captured with a fixed focus digital microscope (Cewei Guangdian, Beijing) (2x objective lens) with a 1600-MP CMOS (DigiRetina 16). High-contrast displacement pattern images were observed by the reflected light (top light source on the microscope). All the displacement pattern images were treated by a grey threshold method to create binary images. Air and liquid saturations can be obtained by an XOR operation between each binary displacement pattern image and the binary image of pore networks. Experimental results showed that the wetting phase can fill the planar pore networks by spontaneous imbibition without threshold displacement pressure. Conversely, when the non-wetting phase (air) displaced the wetting phase (liquid), significant threshold displacement pressure needs to be overcome. The two-phase threshold displacement pressure was determined by the two-phase interfacial tension, contact angle, and pore network structures. The lower the pore network permeability, the higher the threshold pressure. In addition, the results showed that a small amount of dispersed bubbles have relatively slight effect on the air-liquid threshold displacement pressure, while a large number of dispersed bubbles could affect the threshold pressure by changing the through path of the displacing phase. A statistical model was established to estimate the two-phase threshold displacement pressure in the porous media and was verified to be consistent with the displacement experiments.

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Imbibition-Induced Deformation Dynamics in Nanoporous Media: The Interplay of Bangham and Laplace Pressure Effects

Authors: Zhuoqing Li[1]; Juan Sanchez Calzado[1]; Michael Fröba[2]; Patrick Huber[1]

[1] *Hamburg University of Technology*

[2] *University of Hamburg*

Corresponding Authors: juan.sanchez@tuhh.de, zhuoqing.li@tuhh.de, froeba@chemie.uni-hamburg.de, patrick.huber@tuhh.de

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (carbon, silica and polymers) upon spontaneous, capillarity-driven invasion of water. We

find two distinct dynamical regimes. One of them can be quantitatively traced to deformations originating in changes in the surfaces stress at the inner pore walls (dynamic Bangham regime) upon water invasion, whereas the second one results from Laplace pressure effects 1[2][3].

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Flux Regression Neural Networks for Backbone Identification in Discrete Fracture Networks

Authors: Stefano Berrone[1]; Francesco Della Santa[1]; Antonio Mastropietro[1]; Sandra Pieraccini[1]; Francesco Vaccarino[1]

[1] *Politecnico di Torino, Italy*

Corresponding Authors: francesco.dellasanta@polito.it, sandra.pieraccini@polito.it, stefano.berrone@polito.it

Characterization of flow and transport through fractured media in the subsurface is a crucial issue in many engineering applications, e.g. oil and gas extraction or water resources preservation. All these applications require models that can accurately simulate flow through networks of subsurface fractures.
Exact position, size, orientation and hydrogeological properties of all fractures (located hundreds of meters below the ground) can't be determined and therefore statistical representations of fracture networks are introduced and used to simulate flow and transport through fractured media. In this framework the Discrete Fracture Network (DFN) model is largely used.
Due to the probabilistic nature of DFNs, flow and transport characterization in a real fractured medium usually requires a statistical analysis of thousands of DFN generations and simulations. Therefore, in order to speed up simulation processes and to build alternative model reduction methods, for flux regression problems in a DFN it is worth considering the application of machine learning (ML) techniques, and more specifically Neural Networks (NNs) 1. On the other hand, for transport problems in DFNs, one possible technique for speeding up simulations consists in the identification of a backbone of fractures where most transport occurs; also in this cases, due to the expensive computational costs of particle tracking simulations, ML based and graph based methods are preferred [2].
In the framework of DFN with fixed geometry and random transmissivities, we introduce here a method for the identification of single backbones able to approximate the behavior of the exiting flux distributions of the given DFN, varying the transmissivities. In particular, the method used is based on the Layer-wise Relevance Propagation (LRP) algorithm [3] applied to NNs trained for flux regression of DFNs 1, using LRP as a feature selection method to compute the "expected relevance of the fractures"and therefore identifying the backbone.

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Conditions Allowing Steady Two-Phase Flow in Microfluidic Devices

Authors: Afshin Davarpanah[1]; Holstvoogd Jorijn[2]; Simon Cox[1]; William Rossen[3]

[1] *Dept. Mathematics, Aberystwyth U.*

[2] *Dept. of Geoscience and Eng., Delft U. of Technology*

[3] *Delft University of Technology*

Corresponding Authors: afd6@aber.ac.uk, w.r.rossen@tudelft.nl, jholstvoogd@gmail.com, sxc@aber.ac.uk

Microfluidic devices offer unique opportunities to directly observe multiphase flow in porous media. As a direct representation of flow in geological pore networks, conventional microfluidics face several challenges. In three-dimensional (3D) networks, it is thought that two phases can flow steadily, simultaneously, through intertwined pathways without alternating occupancy of locations along the pathways. For large, isotropic, 2D networks, percolation theory prohibits this (1). This is crucial for studies of foam generation in microfluidics (2), for instance, because flow without foam generation (i.e., without fluctuating occupancy of pore throats, i.e. pore connections) would be impossible in such a network.
Microfluidic networks are not strictly 2D, however, in that wetting phase can bridge across the gap between the solid on the two lateral sides of a deep, narrow pore throat while nonwetting phase flows through the center of the throat. This occurs only if the throat is narrower than it is deep. Moreover, if the throat is long and straight, bridging occurs at the same capillary pressure as snap-off, blocking nonwetting-phase flow across the throat.
In this study we examine the conditions under which two phases can flow steadily through a microfluidic network. We assume that the channels have uniform depth, vertical walls, and flat bottom and top surfaces, and that one phase is perfectly wetting of the solid. The curvature of the walls of the throat (viewed from above) can stabilize a bridge against snap-off of the wetting phase. We examine a range of different throat geometries and determine their ability to stabilize bridging without snap-off, using the Surface Evolver program (3) to determine the relationship between interface configuration and capillary pressure. We hypothesize that deep, narrow throats between pillars of tight radius (viewed from above) can stabilize a bridge at capillary pressures too large for snap-off in that throat.
We also examine the conductivity of the pore pathway for each phase to flow, using a network of coordination number 4 as an example. Two-phase flow is possible just above the invasion-percolation threshold for the nonwetting phase. The wetting phase, however, must not only bridge in at least one location, but it must flow around many pore bodies (nodes) occupied by nonwetting phase through narrow channels along the corners at the top and bottom of the pore body. We find that the conductivity of each pore pathway is close to zero, which makes flow without mobilization of phases (4) and subsequent fluctuations in pore occupancy a challenge. The conductivity of the wetting phase is notably small. This suggests that only a small fractional flow of wetting phase can be sustained without forcing accumulation of wetting phase in the network and subsequent fluctuations in pore occupancy. In a study of foam generation at ambient conditions, where the liquid viscosity is 50 times greater gas viscosity, only an extremely small liquid fractional flow is possible in steady flow in such a network. The case is analogous to the case of forcing liquid and gas through a single pore of square cross-section (5).

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Experimental study of CO2/CH4 diffusion coefficient in oil-saturated cores under reservoir conditions

Authors: Yi Zhang[1]; Zerong Li[1]

[1] *Key Laboratory of Ocean Energy Utilization and Energy Conservation of Ministry of Education, School of Energy and Power Engineering, Dalian University of Technology, Dalian, China*

Corresponding Authors: zhangyi80@dlut.edu.cn, lizerong95@126.com

Molecular diffusion is an important mechanism to control the performance of oil recovery processes. The reliable measurement of the diffusion coefficient of CO2 is of great significance for the design and implementation of CO2 enhanced oil recovery (EOR) and carbon capture and storage (CCS) projects. However, relatively few studies on the diffusion coefficient of the CO2-CH4 system in oil-saturated cores. In this study, a series of diffusion experiments of CO2-CH4 system in n-decane saturated Berea core (50mD) were conducted at high pressure (10 to 30MPa) and temperature (333.15 to 423.15K) using pressure-decay technique (PDT), which simulated the reservoir conditions. The CO2-CH4 diffusion coefficients were calculated by a model appropriate for diffusion in porous media based on Fick's law. The results reveal that the diffusion coefficient of CO2 and CH4 decreases correspondingly with the decrease of pressure and temperature. The diffusion coefficient of CO2 and CH4 in the core saturated with oil firstly increases significantly and then the rate of increase gradually slowed down with the increase of temperature and pressure. Compared with the diffusion coefficient of CO2 in oil-saturated, the diffusion coefficient of CO2 and CH4 is much smaller at the same pressure and temperature. Based on the experimental results, an empirical correlation for CO2 and CH4 diffusion coefficient in n-decane saturated core is developed. The experimental results. The experimental results contribute to the study of CO2-CH4 diffusion in cores.

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Tunable interactions during the discharge of a 2D silo

Authors: Louison Thorens[1]; Knut Jorgen Maloy[2]; Mickaël Bourgoin[3]; Stéphane Santucci[3]

[1] *PoreLab - University of Oslo*

[2] *PoreLab*

[3] *ENS de Lyon*

Corresponding Authors: louison.thorens@ens-lyon.fr, k.j.maloy@fys.uio.no

The Janssen effect is certainly one of the most known behavior of granular media, highlighted by the "mass-screening"of a tube filled with grains. Indeed, this grain-specific effect has been vastly studied over the past decades, and seems to be controlled by a unique parameter, the Janssen constant, which depends on the properties of the grains and those of the packing. Moreover, interactions between grains are known to greatly affect the shape and behavior of a granular assembly.
In this presentation we propose to investigate the role of interactions between grains on the overall behavior. To do so, we recreated historical granular experiments to highlight the Janssen effect by using ferromagnetic grains. Under the influence of a magnetic field, these grains acquire tunable momenta, which allowed us to control the Janssen effect in our system. We also performed Discrete Element simulations of ferromagnetic grains to understand the microscopic forces at work, paving the way to a new kind of tunable deformable porous media.

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Diffusion and convection in brain extracellular spaces embedded with perivascular networks

Authors: Vegard Vinje[1]; Miroslav Kuchta[1]; Marie E. Rognes[1]; Timo Koch[None]; Kent-Andre Mardal[2]

[1] *Simula Research Laboratory*

[2] *Simula Research Laboratory, University of Oslo*

Corresponding Authors: meg@simula.no, kent-and@simula.no, vegard@simula.no, miroslav@simula.no, timo.koch@iws.uni-stuttgart.de

The extracellular space (ECS) of the brain is commonly modeled as a porous medium with relatively low permeability. However, perivascular spaces (PVS) surrounding vascular networks may enable fast transport of solutes out of the brain. According to the glymphatic theory 1, cerebrospinal fluid (CSF) rapidly enters the brain along arterial PVS. From there, CSF mixes with interstitial fluid (ISF) and a bulk flow is proposed to occur through the ECS and out of the brain along venous PVS. Several studies [2,3,4] have rather concluded that diffusion is the main transport mechanism within the brain parenchyma. PVS may provide a highway for convective transport to/from the CSF in the subarachnoid space 1. Mathematical models coupling the 3D brain tissue to embedded 1D vascular networks have been used to model perfusion [5]. However, these models are also well suited to study the glymphatic circulation. In this study we used a mathematical model that allowed us to investigate the role of convection and diffusion on transport of solutes in the brain.

First, pressure and velocity fields in the ECS were determined by solving the Poisson equation and Darcy's law for fluid flow in porous media. Dirichlet conditions were set as p = p_a for arterial PVS and p = p_v for venous PVS and the resulting net flow Q through the ECS was computed. Finally, the resistance to flow was computed as R = (p_a - p_v)/Q.
Next, we solved the time dependent convection-diffusion equation with initial condition c(x,0) = c0 for a given solute concentration c0. For the embedded 1D PVS, the concentration was set to 0 under the assumption that these spaces rapidly transport solutes out of the brain. To estimate the time scale of metabolic waste clearance, the mean volume half-life of the solute within the brain was then calculated. Half-life both with and without the convective term was computed.

In the 2D domain adapted from [6], where the average distance between arteriole and venule PVS was 280 micrometers, pure diffusion in the ECS resulted in a half-life of 47 minutes. Adding convection had minimal effect on half-life value. In the 3D domain embedded with PVS surrounding the

entire vascular network, the half-life was estimated to be 3 minutes. In the 2D domain, the resistance of the ECS was computed to be R = 0.57 mmHg/(mL/min). A driving force of only 0.2 mmHg is thus sufficient to drive Q = 0.2/R = 0.35 mL/min, a flow rate similar to CSF production.

Provided that PVS act as CSF highways 1, our preliminary results suggest that diffusion is sufficient for clearance within ECS. In particular, the almost space-filling structure of the network enable much faster clearance than what has been obtained with simplified models with only few vessels. Although permeability and velocities in the ECS are known to be relatively small [3], the extensive perivascular network permeating it ensures that pressure driven ISF flow from arteriole PVS to venule PVS has a low resistance.

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A variation free approach for free energy minimization in density functional theory.

Author: Yuriy Kanygin[1]

Co-authors: Irina Nesterova [1]; Pavel Lomovitskiy [1]; Aleksey Khlyupin [1]

[1] *Moscow Institute of Physics and Technology*

Corresponding Authors: lomovitskiy.pv@cet-mipt.ru, khlyupin.an@cet-mipt.ru, irina.nesterova@phystech.edu, yuriy.kanygin@phystech.edu

A large number of natural or technological processes (hydrocarbons flow in coal and shale, capturing and storage of CO2, fluid separation, etc.) are related to fluids in the pores of nanometer scale. Fluids can be well described at this scale by density functional theory (DFT). DFT is actively developed and used for investigating thermodynamic properties in confinement systems [1, 2]. To find the equilibrium state of a system, it is necessary to analytically calculate the free energy functional variation. For many systems and geometries, it is nearly an impossible task. Besides, a slight change in the system results in the need to completely recalculate variations. Further, one has to calculate the equilibrium fluid density via the simple iteration method [3] or matrix-free algorithm [4].

The equilibrium density, which minimizes the free energy potential, can be represented as a basis functions expansion. To obtain such expansion, we built a finite set of densities of different fluids under different thermodynamic conditions. It is important to note that the dataset does not contain the solution to our problem. Then the principal component analysis (PCA) was applied to compute the most significant basis functions, and the answer is sought as the superposition of these functions. This approach provides expansion with negligible approximation error and gradually reduces the number of optimized parameters, also it gives an advantage in the speed-up of nonlinear terms calculation.

To use a variation-free approach, we rewrite the problem of finding the equilibrium density as an optimization problem. As the objective function, we use the free energy functional, which contains information about thermodynamical properties and molecular structure of the system. Our goal is to find the best set of coefficients of the density expansion, that would minimize the functional of free energy. We apply the widely known zero-order black-box stochastic optimization methods such as genetic algorithm (GA), particle swarm optimization (PSO) and separable natural evolution strategies (SNES) in our research. These algorithms help avoid the analytical calculations of the variation and seek for the global minimum of the free energy functional.

The key objective of this work is an elimination of the necessity to analytically calculate the variations of the free energy functional and to recount them each time for different systems with different thermodynamic potential. We solved a problem of finding the equilibrium density distribution of Ar and N2 in carbon slit pore at temperatures T = 87.3, 77.4 K with different width (2, 4, 6, 8, 10 nm) and relative pressure (6e-5, 2e-3, 6e-2, 0.9, 1). We chose 10-4-3 Steele potential as wall potential. The parameters of solid-fluid and fluid-fluid interactions were chosen according to 1. Results are in good agreement with the standard solutions and the acceleration in the calculations is up to 20%.

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Evaporative cooling in fuel cells: Estimating effective conductivity in gas diffusion layers

Author: Sarah van Rooij[1]

Co-authors: Mirco Magnini [2]; Sophia Haussener [3]

[1] *Ecole Polytechnique Federale de Lausanne*

[2] *Department of Mechanical, Materials and Manufacturing Engineering, University of Nottingham, U.K.*

[3] *École Polytechnique Fédérale de Lausanne*

Corresponding Authors: sophia.haussener@epfl.ch, mirco.magnini@nottingham.ac.uk, sarah.vanrooij@epfl.ch

The utilization of evaporative cooling in the gas diffusion layers (GDLs) of fuel cells can efficiently dissipate the heat produced by high power density fuel cells, thus leading to an economically more competitive PEM fuel cell. The highly porous GDLs offer a large surface area, allowing to cope with

larger heat fluxes and leading to larger evaporation rates. Because of the computational requirements necessary to design a pore-scale GDL model, a macroscopic approach to the multi-physical problem of evaporative cooling is often preferred. The porous media of the partially saturated GDL can be modelled through effective medium theory, using a volume-averaging approach [i]. In this work, we focus on the effective thermal conductivity.

A three dimensional partially saturated geometry was digitalized based on the exact GDL microstructural data obtained from X-ray tomography (resolution $2.3\,\mu\mathrm{m}$), considering a representative elementary volume ($0.6 \times 0.6 \times 0.3\,\mathrm{mm}^3$). The model was numerically discretized into an unstructured tetrahedral volume mesh, where each phase (water, fibers, gas mixture) was defined separately with well-defined interfaces.

Illustration of the partially saturated GDL, where the water evaporates and mixes with the carrier gas. The close-up look on the bottom right shows a schematic of the GDL considered in this work, partially saturated, where the bulk properties of the 3 phases are defined 1

The energy equation was solved in ANSYS Fluent, where fixed temperatures were applied on both side of the model. The governing equations for the determination of the effective conductivity in a porous medium are based on a one-equation averaging model, which assume local thermal equilibrium [ii]. The GDL porous media is considered as anisotropic material, assumed orthotropic as the in-plane directions are equal.

The effective conductivity was calculated in the sample at different conditions such as porosity and capillary pressure, as well as for a large range of bulk thermal conductivities for the solid, liquid and gas materials.

For specific cases, the addition of the evaporation of the water was implemented in the model. The mass and momentum conservation equations as well as the species transport equation were solved, in addition to the energy equation. Evaporation at the liquid-vapor interface was modelled using kinetic theory, based on the Hertz-Knudsen-Schrage equation [iii] and implemented via self-defined routines.

The change in effective conductivity as a result of the addition of evaporation where compared to the results obtained without phase-change were calculated and compared. The numerical model confirmed a decrease of the effective conductivity when evaporation is considered because of the latent heat removal. Different types of pores, saturation levels and material properties were explored.

The numerical multi-physics model provides a combination of effective conductivity values to be used as prediction of heat transfer in GDL structures. These effective properties can be used in continuum models of complete fuel cells.

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Joint influence of in-situ stress and fracture network geometry on heat transfer in fractured geothermal reservoirs

Authors: Xiaoguang Wang[1]; Chuanyin Jiang[2]; Qinghua Lei[3]; Zhixue Sun[2]

[1] *Hydrosciences Montpellier*

[2] *China University of Petroleum - East China*

[3] *ETH Zurich*

Corresponding Authors: x.wang0127@gmail.com, chuanyin_jiang@foxmail.com, qinghua.lei@erdw.ethz.ch

We quantitatively investigate the superimposed influence of geometrical properties and geomechanical deformations of two-dimensional fracture networks on heat transfer in fractured geothermal reservoirs. The reservoir model consists of rock matrix with uniform properties and natural fractures following power law length scaling. We model its thermo-hydro-mechanical behavior based on sequentially linked solvers that resolve the solid deformation, fluid flow and heat transport processes. The fracture aperture is spatially variable and dependent on the stress loading conditions, based on which stress-dependent fluid flow is further simulated. Our numerical results show a good correlation between the heat extraction efficiency and the fracture network connectivity. The connectivity seems to be a prerequisite for geomechanical factors to impact heat transfer. Depending on the hydraulic boundary condition, the stress loading may lead to different geothermal responses: under a high hydraulic gradient, an increased stress ratio results in a decrease in the heat extraction efficiency; in contrast, under a low hydraulic gradient, an increased stress ratio corresponds to an enhanced heat production. The observed effects of in-situ stress and fracture network geometry on heat transport are quantitatively characterized by a dimensionless analysis using the fracture-matrix Péclet number, which is defined as the ratio of convection timescale in the fracture to conduction timescale in the matrix. Our research findings have important implications for understanding the heat exchange performance of fractured rocks in geothermal reservoirs naturally subjected to complex in-situ stress conditions.

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Measuring the deformation of porous media in response to hydraulic pressure.

Authors: Martin Stolar[1]; yaniv edery[1]; Tajudeen M. Iwalewa[2]; James R. Rice[3]

[1] *Technion*

[2] *Harvard*

[3] *Harvard*

Corresponding Authors: tajlanre1@seas.harvard.edu, rice@seas.harvard.edu, yanivedery@gmail.com, mstolar@campus.technion.ac

Induced seismicity or earthquakes caused by human activity have become more frequent in the last decade and their occurrence is expected to increase due to anthropogenic activities such as hydraulic fracturing, wastewater injection and CO2 sequestration. Therefore, deeper understanding of parameters ruling the starting mechanism of this earthquake is essential. The elementary parameters controlling fractures are known to be pore pressure and shear stress. Naively, the pore pressure increase is the direct result of fluid injection. However, this propagation follows the permeability variation and induce microfractures which funnels the flow towards the fault. Understanding the permeability effect and micro-fractures on pore pressure increase will improve risk assessment for induced seismicity.

In our experiment, sub-surface porous media are modeled using polymethylmethacrylate (PMMA) beads with a diameter of around 30 μm. Layers of these beads are chemically sintered together in a rock-like structure. The refractive index of this structure is matched with the wetting and non-wetting fluid. Therefore, it is possible to visualize the replacement of one fluid with another using the confocal microscope. In the experiment, the flow rate of the invading phase is controlled by the pressure imposed on it. Parallel to this it is possible to follow the plume in the porous media

on the micro-scale. An important observation showed that the invading phase deforms the domain, and locally the domain permeability, leading to a focusing of the plume invasion towards the outlet.

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Evaluation of CO2 enhanced recovery potential as pre-pad in tight reservoir compared with slickwater

Author: Liyao Fan[1]

Co-authors: Yuliang Su [1]; Lei Li [1]; Mingyu Cai [1]; Zheng Chen [1]; Chengwei Wang [1]; Xiaogang Gao [1]

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

Corresponding Authors: cmy9724@163.com, chenzheng190313@163.com, gaoxiaogang1@126.com, wangchengwei_upc@163.com, lei.li@upc.edu.cn, suyuliang@upc.edu.cn, fanliyao_upc@163.com

Slickwater is one of the most commonly used fracturing fluids, however it consumes amount of water, induces reservoir damage and flows back difficultly. CO2 is friendly to tight reservoir, which can enhance oil recovery and facilitate fracturing fluids backflow by interacting with oil. Furthermore, the injected CO2 will be adsorbed and permanently stored in the formation, alleviating the greenhouse effect [1-2]. Nevertheless, researches on the enhancement recovery potential of CO2 as pre-flush injecting fluid before fracturing are quite few [3-4]. Therefore, we quantitatively investigated the stimulation potential of CO2 prepad for tight reservoirs by experimental and numerical methods.

First, the influence of CO2 on the volume of crude oil was studied through Constant Composition Expansion. Meanwhile, the displacement efficiency of CO2 was calculated by laboratory experiments. Then, comparison experiments with slickwater flooding were also conducted. Next, a conceptual model was established by using CMG commercial software, considering CO2 dissolving, and the resulted miscible process and oil swelling. We injected CO2 followed by water in the model to simulate CO2 pre-pad. As well as, the effect of CO2 on stimulation and fracturing fluid flowback was quantitatively evaluated. Finally, CO2 injection rate, CO2 injection volume and soak time for fracturing operation was obtained by Response Surface Method, providing a vital guidance for oil-field.

The results show that: (1) When 25% mole fraction of CO2 injected into crude oil, the volume factor and swelling factor of crude oil increased by 19% and 33%, respectively. That indicated CO2 can make crude oil fully swelling and remarkably increase its elastic energy; (2) The displacement experiment displayed that the displacement efficiency of CO2 is four times higher than slickwater, and the oil breakthrough time of CO2 flooding is just one quarter slickwater. Combined with the result of Nuclear Magnetic Resonance experiment, it is showed that the displacement efficiency of slickwater is confined by the pore size distribution of core. While the displacement efficiency of CO2 is not affected by the pore size distribution of core because of small molecule and easy diffusion ability of CO2. Thus, the oil recovery by injecting CO2 into reservoir is notable and widely applicable; (3) The numerical simulation showed that the recovery factor of CO2 as prepad is 9% higher than slick water. The flowback rate of the fracturing fluid when injecting CO2 prepad is 1.4 times greater than injecting slickwater, because fracturing fluid is easier to flowback after the full interaction between CO2 and crude oil during the soak stage. That indicates CO2 is an effective and promising to enhance recovery for tight oil. (4) At last, Response Surface Method was applied to optimize multiple operating parameters. It turned out that best CO2 injection rate is 4m3/min, optimal CO2 injection volume is 500m3, and proper soak time is 9 days . According to the research, the effect of CO2 in enhancing oil recovery and improving fracturing fluid backflow outperforms slickwater. CO2 as prepad injecting fluid before fracturing has a wide prospect to stimulate tight reservoirs.

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Novel Method for Improving Injectivity of Polymer solution in Porous Media

Author: Mohsen Mirzaie Yegane[1]

Co-authors: Julia Schmidt [1]; Fatima Dugonjic-Bilic [2]; Benjamin Gerlach [2]; Pacelli Zitha [3]

[1] *Delft University of technology*

[2] *TouGas Oilfield Solutions*

[3] *TU Delft*

Corresponding Authors: p.l.j.zitha@tudelft.nl, m.mirzaieyegane@tudelft.nl

Synthetic high molecular weight polymers have been utilized for enhanced oil recovery (EOR) applications; however, improving their injectivity in emulsion form (i.e. dispersion of hydro-gels of water-soluble synthetic polymer in oil) remains an important issue for field applications. Commercially available polymers used for EOR are commonly poly-disperse, i.e. have a broad molecular weight distribution (MWD). The high-end members of the polymer MWD cause injectivity problems because the polymer molecules are too large to enter the porous media which leads to clogging pore throats and consequent injectivity decline.

The purpose of the present work is to improve the polymer injectivity by deliberately conditioning the polymer solutions. We have developed a series of processing techniques to condition a polymer solution in high total dissolved solids (TDS) content brine prior to injection into porous media. The investigated polymer solution contained an acrylamide-based co-polymer inverse emulsion and an inverter surfactant. The polymer solution was sheared with two agitators, a disperser and Ultra-Turrax, at different intensities and with a pressure-driven flow into a thin capillary in order to reduce the size of the largest polymer chains (i.e. to cut the high-end of the MWD) and disentangle the polymer chains while maintaining its viscosifying power. The injectivity of such differently sheared solutions in porous media was assessed by performing filtration and sand-pack flooding tests.

Our experiments established a master curve of viscosity and screen factor dependencies on accumulated energy during pre-shearing showing that both viscosity and screen factor approach asymptotic values. This is explained by the elimination of the high end of the MWD with pre-shearing. Such master curve was independent of shear origin.

After pre-shearing, the filtration behavior of polymer solution and its injectivity in sand-packs improved significantly. Polymer solutions sheared with a disperser at an energy input of 15 MJ/m3 improved the injectivity gradient (e.g. the ratio of the resistance factor over 30 pore volumes injected) from 3.7 to 1.6, while the viscosifying power was reduced by only 2%. To reach the same injectivity improvement with Ultra-Turrax, an energy input of 31 MJ/m3 were required, which reduced the viscosity by 11%. Shearing the solution using a capillary at an energy input of 50 MJ/m3, did not reduce the injectivity gradient while viscosity was reduced by 19%. Despite the existence of rheological master curves, the study showed that no injectivity master curves exist. This indicates that the injectivity behavior cannot be determined by merely looking at the rheological properties such as viscosity and screen factor, making the flooding tests in porous media inevitable.

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Wormholing and channelling: impact of heterogeneity on dissolution regimes in porous media using pore-scale direct numerical simulation

Author: Julien Maes[1]

Co-authors: Hannah Menke [1]; Alexandros Patsoukis Dimou [2]; Sebastian Geiger

[1] *Heriot-Watt University*

[2] *Heriot Watt Univesrity*

Corresponding Authors: ap92@hw.ac.uk, s.geiger@hw.ac.uk, h.menke@hw.ac.uk, j.maes@hw.ac.uk

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 particular conditions of the injection process as well as the mineral properties strongly influence the resulting dissolution pattern, leading to compact, uniform, wormholing, or channelling 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 numerical model, based on the OpenFOAM toolbox, is presented and validated by comparison with experimental results. A series of numerical simulations are then performed on stochastically generated synthetic 2D micromodels with increasing pore space heterogeneity. For each model, the influence of flow and reactive conditions on the local dissolution is characterized and the boundaries between the different dissolution regimes are obtained. 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. In addition, we characterise the difference between uniform dissolution regime, that occurs at low Damköhler and Péclet numbers, and channelling, that occurs at low Damköhler and high Péclet number. We present a novel way to measure pore-space heterogeneity which we then use to add a third dimension to the traditional conceptual model of dissolution regimes within the Damköhler-Péclet space.

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Direct pore-scale numerical simulation of two-phase flow and reactive transport using the Volume-Of-Fluid method

Author: Julien Maes[1]

Co-authors: Cyprien Soulaine [2]; Sebastian Geiger

[1] *Heriot-Watt University*

[2] *Stanford University*

Corresponding Authors: s.geiger@hw.ac.uk, cyprien.soulaine@gmail.com, j.maes@hw.ac.uk

Multiphase multispecies transport is an essential field of studies for a wide range of subsurface applications including oil and gas production, CO2 storage and contaminant hydrology. Modelling of these processes is challenging due to the discontinuity of material properties at the interface and interfacial boundary conditions resulting from surface tension force and mass transfer. Currently, there are three main barriers into accurate and robust simulations of pore-scale multiphase transport process: (1) numerical error due to the inaccurate modelling of surface tension force at low capillary number, (2) excessively large CPU time due to time-step restriction induced by capillary waves propagation at low capillary number and (3) accurate modelling of mass transfer at reactive interface. In this work, we present recent advances that allow us to perform numerical simulations at any capillary number, in particular as low as we want. Our numerical model is applied to simulate the dissolution of CO2 bubbles in 3D printed micromodels.

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Fracture pore network model: efficient pore scale modelling of fluid flow in fractured porous media

Authors: Chenhui Wang[1]; Kejian Wu[1]; Gilbert Scott[1]

[1] *Aberdeen University*

Corresponding Authors: r01ggs16@abdn.ac.uk, r02cw17@abdn.ac.uk, kejian.wu@abdn.ac.uk

Fluid flow through fractured porous media occurs commonly in the subsurface such as the hydrocarbon flow in the fractured reservoirs. However, current discrete fracture modelling methods that simulate the transport processes in fractured porous media, using finite element method and lattice Boltzmann method, are computationally expensive. We have developed a new fracture pore network model (FPNM) to efficiently simulate the fluid flow properties in fractured porous media associated with the pore matrix.

We extend the idea of pore network models (PNM) (Blunt, 2017) to fracture pore network model by adding a new explicit fracture element in addition to the pore matrix that is traditionally idealised as pore body and pore throat elements. The fracture element is simplified as an ideal planar cuboid with properties of aperture, width, length and orientation. The complex pore structure can be represented by a topological network of pore bodies (nodes) and fractures, which are connected by pore throats (bonds). These three elements within the FPNM are assigned with the key features of pore structure.

The fluid flow between the fracture and the matrix in the FPNM with a single fracture is investigated first. The results are compared with finite element simulation by using COMSOL Multiphysics® (AB, 2018). The FPNM is then extended to include multiple non-intersecting fractures consequently. Pore networks with fracture elements were extracted from a couple of test images and the results are compared with finite element simulation in terms of permeability, flow rate and pressure. A reasonable agreement was achieved which demonstrates the value and efficiency of the fracture pore network models.

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Modelling the drying shrinkage of porous materials incorporating capillary and adsorption effects

Authors: GINGER EL TABBAL[1]; Patrick Dangla[2]; Matthieu Vandamme[3]; Marina Bottoni[4]; Sylvie Granet[4]

[1] *EDF R&D - LABORATOIRE NAVIER*

[2] *Université Paris-Est Laboratoire Navier (UMR 8205) CNRS, École des Ponts Paris Tech, IFSTTAR, France*

[3] *Ecole des Ponts ParisTech*

[4] *EDF R&D*

Corresponding Authors: marina.bottoni@edf.fr, matthieu.vandamme@enpc.fr, sylvie.granet@edf.fr, patrick.dangla@ifsttar.fr, ginger.el-tabbal@edf.fr

Durability of concrete structures is a major research area for EDF. This research focuses in particular on the drying behaviour of a high performance concrete used as a shell for nuclear waste packages. The package of interest will be conserved in a surface interim storage facility and then disposed off at CIGEO [10] (i.e. the future underground disposal facility for long term radioactive waste in France). During the interim storage phase, the concrete shells will be submitted to a relative humidity that could be lower than 50% and a relatively high ambient temperature (attaining 50℃).
In order to estimate the drying evolution of the shell under these conditions, the thermo-hydro-mechanical behaviour of the concrete should be correctly modelled. The current work focuses on deriving a suitable poromechanical model for the prediction of the corresponding drying shrinkage strains and stresses.
When a porous material (such as concrete) is subjected to drying, corresponding strains will occur. A restrainment of the latter induces a development of internal stresses that could eventually cause material cracking. Subsequently, a proper poromechanical model is needed to predict those stresses/strains and hence prevent the appearance of cracks. Different models 1,[2],[3] based on the concepts of capillary or disjoining pressure are found in the literature. Nevertheless, it has been shown[4] that those models failed to describe the evolution of drying shrinkage strains for a relative humidity lower than 40% - 50%. This deficiency can be linked to the fact that those models neglect the presence of adsorbed water on the surface of desaturated pores.
In this work, a model based on a thermodynamical approach describes the drying of unsaturated porous media for a large range of relative humidity. The derived model accounts for various contributions that include: the capillary pressure, the water adsorption, and the Shuttleworth effect [5] which recognizes that at an elastic solid interface, the surface energy is different from the surface stress. Most of the input parameters of the model, related to the evolution of the unsaturated pores volume and surface, are assessed by the B.E.T[6] and the BJH techniques[7]. The remaining input parameters, related to the hygro-mechanical coupling (such as the Biot coefficient and a parameter governing the magnitude of the Shuttleworth effect) are fitted on experimental drying shrinkage strains.
The model was validated by comparing the predictions to experimental drying shrinkage strains data found in the literature for different porous materials (hardened cement paste, high performance concrete and Vycor glass). The obtained results are quite satisfactory. In particular, when compared to other models found in the literature 1 [8], this model appears to be exclusively able of displaying the transition at a certain relative humidity between the contribution of the capillary pressure and that of the adsorption.
Furthermore, the new model is validated by experimental drying shrinkage tests performed in the internal laboratories of EDF on a high performance concrete. The model has been implemented in the EDF finite element software Code_Aster[11] and will be used to describe the drying behavior nuclear waste packages.

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Incremental petrophysical characterization of carbonate rocks using µCT box counting fractal analysis for upscaling purposes

Authors: Tatiana Lipovetsky[1]; Luca Moriconi[2]; Behzad Ghanbarian[3]

Co-authors: Eduardo Ribeiro [1]; Mateus Ramirez [1]; Elizabeth May Pontedeiro [1]; Martinus van Genuchten [4]; Paulo Couto [1]

[1] *LRAP/UFRJ*

[2] *IF/UFRJ*

[3] *Kansas State University*

[4] *Federal University of Rio de Janeiro*

Corresponding Authors: mateusgr@poli.ufrj.br, moriconi@if.ufrj.br, pcouto@petroleo.ufrj.br, rvangenuchten@hotmail.com, ghanbarian@ksu.edu, tatianalipovetsky@petroleo.ufrj.br, bettymay@petroleo.ufrj.br, eduardo.ribeiro@nidf.ufrj.br

Petrophysical characterization of oil-bearing rocks is crucial for improving petroleum recovery. Among other techniques such as NMR (Nuclear Magnetic Resonance) or direct measurements of capillary pressure –saturation (Pc-S) curves, fractal modelling of the pore structure based on microcomputerized tomography (µCT) images is an important ingredient for the petrophysical description of rock formations and, ultimately, for improved recovery of the fluids of interest.
Natural porous media are frequently classified as fractal objects, meaning that some of their statistical geometric features, such as the volume or pore radii distributions, can be well described using scaling power-laws.For homogeneous rock samples, one expects that the number of pores which have linear dimensions smaller than s scales as N(s) = as^-D, where D is the sample's fractal dimension.
Many carbonate rocks, such as the ones present in the Brazilian Pre-salt, generally exhibit multiporosity properties. Direct measurement of their Pc(S) and relative permeability curves using HYPROP and WP4C laboratory tests, and subsequent analysis of the data in terms of the van Genuchten hydraulic functions, showed compatibility with the NMR data, while very much confirming their dual-porosity behavior.
The present work addresses a critical issue about the application of the usual box counting methodology to the study of carbonate rocks within the context of multifractal analysis. The coexistence of two or more porous structures inside a formation dictates how fluids flow through the rocks, as well as how the pore structure affects rock-fluid and fluid-fluid interactions. The fractal dimension of µCT box counting can be compared with the fractal dimension obtained from NMR data. Being able to characterize the multi-porosity nature of the system with the fractal approach allows one to formulate upscaling predictions that provide certainty and feasibility to the investigated cores, while minimizing the need for costly and time-consuming analyses of large-scale field tests.

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Adaptive Virtual Element Method for simulations of flow in fractured media

Authors: Andrea Borio[1]; Stefano Berrone[1]; Alessandro D'Auria[1]

[1] *Politecnico di Torino, Italy*

Corresponding Authors: alessandro.dauria@polito.it, andrea.borio@polito.it, stefano.berrone@polito.it

One of the main issues in devising robust methods for the simulation of physical phenomena in fractured media is the handling of geometrical complexities, that can make it difficult to generate a good quality computational grid. Moreover, the computational efficiency of simulations is crucial, since they are usually performed on many configurations of the subsoil, generated randomly from physical properties distributions.
This talk deals with an adaptive strategy, based on the Virtual Element Method, for the simulation of flow in a fractured medium, represented as a 3D Discrete Fracture Network. Starting from a minimal polytopal grid and using suitable a posteriori error estimates 1, the adaptive process is able to identify and refine only those fractures where the flow is more relevant, thus containing the number of degrees of freedom and the computational cost. Efficient refinement strategies for polytopal grids, able to preserve mesh quality, are also presented [2].

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A fractal model for shale gas apparent permeability

Authors: Fanhui Zeng[1]; Chao Wen[1]; Jianchun Guo[2]; Qiang Zhang[2]; Jianhua Xiang[3]

[1] *Southwest Petroleum University*

[2] *State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu, China*

[3] *Engineering Technology Research Institute, Chengdu, China*

Corresponding Authors: guojianchun@163.com, 1154346290@qq.com, wenchaockol@163.com, zengfanhui023024@126.com, xiangjh@petrochina.com.cn

The organic capillary and the inorganic capillary together constitute the shale pore microstructure. The gas in the organic capillary is mainly free gas and adsorbed gas, while the gas in the inorganic capillary is mainly free gas and water film. What's more, the stress sensitivity can cause significant changes in pore characteristics of shale during the development of shale gas, making it difficult to characterize the complex seepage mechanism by the existing permeability model. Based on Hagen-Poiseuille equation and shale tortuous capillary bundle model, this paper establishes a model of apparent permeability of shale, considering the fractal model which can more realistically display the pore microstructure of shale reservoirs. The validity and rationality of this model has been demonstrated by experimental data. It is found that the stress sensitivity will increase the tortuosity fractal dimension and decrease the pore fractal dimension. Meanwhile, it also affects the desorption of adsorbed gas in organic capillary and the thickness of water film in inorganic capillary, resulting in an increase in the apparent permeability of organic capillary and decrease in the apparent permeability of inorganic capillary. In addition, factors such as the ratio of maximum and minimum diameter of shale capillary also have a great influence on the apparent permeability of shale. This paper provides an analytical model to predict the apparent permeability of shale and a theoretical guidance for the development of shale gas.
Keywords: shale gas; fractal porous media; apparent permeability; stress sensitivity; slippage effect

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Evaluation of Gas Adsorption Behavior in Nanoporous Shale Using Simplified Local-Density Model Integrated With Cylindrical and Slit Pore Structures and Pore Size Distribution

Author: Yu Pang[1]

Co-authors: Sen Wang [2]; Shengnan Chen [1]

[1] *University of Calgary*

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

Corresponding Authors: snchen@ucalgary.ca, fwforest@gmail.com, yu.pang1@ucalgary.ca

Simplified Local-Density (SLD) model has been widely used to describe the adsorption isotherm in shale. However, the constraints ascribed to the slit pore geometry and constant pore width fail to represent the heterogeneous pore structure in shale formations. In this study, we incorporate the cylindrical and slit pore structures and the pore size distribution (PSD) into the SLD model to improve the characterization of complex pore networks in shale.
In this study, the SLD model with the cylindrical pore structure was developed to account for the curvature effect on gas adsorption. The validity of such a model was examined by comparing the predictions of the SLD model with a cylindrical pore to the simulation results via the grand canonical Monte Carlo (GCMC). Furthermore, the PSD ranging from micro- to mesopores was determined based on the carbon dioxide and nitrogen adsorption measurements, which was interpreted as a combination of log-normal distributions. Finally, the functions for the PSD were integrated into the SLD models with slit and cylindrical pore structures.
The agreement between the SLD model and the GCMC simulation is found. Unlike the GCMC simulation which is limited to a single nano-tube or slit, the developed SLD model is able to precisely depict the measured adsorption isotherm of methane on Wolfcamp shale core sample. The results of this study indicate that both pore structure and PSD have tremendous influences on gas adsorption in nanoporous shale. The amount of adsorbed gas in the cylindrical pore structure is more than 20% lower than that in the slit pore structure when the pore size, surface area, and adsorption energy parameter are set to be equivalent.
The SLD model equipped with the pore structure and PSD features is capable of evaluating the adsorption behavior over the entire pore size range with different pore geometries, which greatly enhances the applicability of the SLD model to the nanoporous media with complex pore networks and sheds light on the relationship between pore structure and gas adsorption capacity of the shale formations.

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Smart Capillary Barrier-Wick: A Self Irrigating Technique Inspired by Nature for Home Gardens in Arid Zones

Author: Ahmed Al-Mayahi[1]

Co-authors: Said Al-Ismaily [1]; Ali Al-Maktoumi [1]; Hamed Al-Busaidi [1]; Anvar Kacimov [1]; Rhonda Janke [2]; Johan Bouma [3]; Jirka Šimůnek [4]

[1] *Department of Soils, Water and Agricultural Engineering, Sultan Qaboos University, Al-Khoud 123, Oman*

[2] *Department of Crop Sciences, Sultan Qaboos University, Al-Khoud 123, Oman*

[3] *Emeritus Professor Soil Science, Wageningen University & Research, the Netherlands*

[4] *Department of Environmental Sciences, University of California, Riverside, CA 92521, USA*

Corresponding Authors: almayahi.squ@gmail.com, jsimunek@ucr.edu, rhonda@squ.edu.om, ali4530@squ.edu.om, hbusaidi@squ.edu.om, anvar@squ.edu.om, esmaily@squ.edu.om, johan.bouma@planet.nl

As in many arid climate cities, home gardeners in Muscat, Oman are discouraged to garden due to water scarcity and heat stress. Additionally, 70% of them irrigate their gardens with a desalinated drinking water which ultimately increases their water bills (Al- Mayahi et al., 2019). In this study, we present an engineered capillary barrier-wick (SCB-W) irrigation system for arid zone gardens

that was designed from the prototype of a smart capillary barrier (SCB) structure discovered inside the reservoir bed of Al-Khoud dam, Oman (Al-Ismaily et al., 2013). The SCB-W is made of a composite soil of staggered silt loam blocks (top and bottom layers) surrounded by thin sand sheaths irrigated by a sand-filled wick cylinder. Topology of the pore level fluid flows is similar to one in hydro-fracked formations (Blunt, 2017), although the sheath acts not as a damper keeping the aperture against a geostatic pressure but as an anti-evaporation "proppant"preserving soil moisture in the blocks for plant-roots transpiration.
We carried out pot experiments in the field and HYDRUS (2D/3D) modelling with hysteresis in the capillary curves and non-hysteretic phase permeability function, to study cyclostationary soil-water distribution and evaporation under the SCB-W compared to a control (homogenous soil irrigated by the same wick system, HW). We also investigated the effect of the wick diameter (2.54 cm vs 1.27 cm) on the imbibition-drainage cycles. The experiments were run in two consecutive phases: phase II differed from phase I by having a sand mulch on top of the substrates. The volumetric water content θ in each substrate was measured by installing four ECH2O EC-5 sensors, two at the top and two at the bottom part, connected to a datalogger Em50 (Decagon Devices). Matching between simulated and measured θ was evaluated by the root mean squared error (RMSE), the Nash-Sutcliffe coefficient (NSE), and the Willmott index (d). Data were analyzed using a three-way repeated-measures ANOVA on Datadesk 8.1 (Data Description Inc), where p-values <0.05 were considered significant, and demonstrated that HYDRUS simulated θ was in a good agreement with the measured one ($0.001 < RMSE < 0.062$, $0.508<NSE<0.999$, and $0.970<d<0.999$). Based on the field experiments and modelling, SCB-W increases two times the wetting dynamics of the soil substrate than the HW during the wetting cycles in both phases ($P<0.0001$). Decreasing the diameter of the wick-cylinder prolonged the wetting time by 1 and 3 days for the SCB- W and HW, respectively, nevertheless, still SCB-W wets the substrate two-times faster compared to HW ($P<0.0001$). SCB- W had 44.3-52.4% higher θ in its bottom part than HW during the drying cycles ($P<0.0001$). Placing a sand mulch layer on top of both substrates decreased evaporation, hence increased θ by 20-38.9% during the drying cycle ($P<0.0001$). Future work will include theoretical investigation of Stokes microhydrodynamics in Blunt's (2017) menisci-bounded polygonal channels and practical testing of the water use efficiency of SCB-W with active roots of ornamental plants.
Keywords: Wick irrigation system; HYDRUS (2D/3D); Capillary barrier; Engineered soil; Water scarcity; Urban gardening.

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Distribution of oil in shale formations and its effects on kerogen nano-structural properties

Authors: QIAN SANG[None]; XINYI ZHAO[None]; MINGZHE DONG[None]

Corresponding Author: 20190005@upc.edu.cn

Shale oil formation are complex and heterogeneous systems that contain both inorganic minerals and organic material (kerogen). The inorganic minerals are hydrophilic, and the kerogen is hydrophobic. Due to their different wetting abilities, the fluid storages of kerogen and inorganic mineral are different. Kerogen only contains oil that stays in free, adsorbed and dissolved forms, while inorganic minerals contain both oil and water in free and adsorbed forms. It is important to characterize the distributions and contents of water and oil in shale reservoirs because oil and water distributions

have significant impacts on two-phase flow in shale. Based on single-phase saturation process, we define maximum inorganic and organic oil saturations and porosities in shale. Two types of vacuum-imbibition tests - water imbibition and oil imbibition - on 20 shale oil rock samples were performed to distinguish the two saturations. For the shale rock samples tested, the oil content in organic matter ranges from 6% to 55% of the total oil content. Vacuum-imbibition experiments have shown significant contrast in water saturation and oil saturation. The final oil imbibed volume is much higher than the final water imbibed volume. Based on the molecular model of kerogen and inorganic materials, we conducted molecular dynamics simulation to model the imbibition tests of water and oil in shale samples. Results show that oil and water can enter different media: water molecules can only enter in the inorganic mineral pores and barely enter into the kerogen matrix, while the oil molecules can enter not only the pores within kerogen but also the intermolecular spaces inside kerogen. About 30% to 50% of the total oil can penetrate into the intermolecular spaces of kerogen, representing the dissolved oil in kerogen. Furthermore, the volume of kerogen can expand during oil absorption process, accounting for the swelling of kerogen. As a result, the surface area, porosity, and pore size of kerogen increase with oil uptake. The results of this study provide basic understanding of the storage of oil in shale and fundamental knowledge for multiphase flow and oil recovery in shale oil reservoirs.

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Deformation of kerogen and its effects on oil flow in shale

Authors: XINYI ZHAO[None]; QIAN SANG[None]; YAJUN LI[None]; HOUJIAN GONG[None]; MINGZHE DONG[None]

Corresponding Authors: 20190005@upc.edu.cn, 498673169@qq.com

Shale oil reservoirs are complex formations containing organic matter (OM) and inorganic content. Oil in shale includes free oil within inorganic pores and ad-/absorbed oil within kerogen. Due to the molecular interactions between oil and OM, the mechanism of oil transport in shale is more complicated than that in other formations, and remains unclear. In this study, we conducted oil flow experiments in shale and tight sandstone core samples by recording flow rates and pressure drops with testing time. Under constant injection pressure condition, tests with shale samples showed an increase-and-decrease fluctuation in production rates before attaining a steady state flow. This type of fluctuation in the flow rates was not observed in the tests with tight sandstone samples. Analysis of the experimental results using the theory of interactions between oil molecules and kerogen showed that the oil saturated kerogen needs to expand to an extent so that oil within the kerogen can overcome the interaction and be released from the kerogen. The permeability of kerogen increases during the deformation process. A model is proposed for describing the relation between the permeability and the volumetric expansion of kerogen. Numerical simulation with the proposed model can successfully match the experimentally measured oil production curves. Field scale modeling indicates that 1) high content of kerogen can increase the total elastic recovery of shale formations; 2) there is a critical pressure drop from the initial pressure within kerogen for triggering the release of the absorbed oil from kerogen; and 3) short distance between the factures can increase oil release rate in kerogen. These results provide a better understanding of the flow mechanism of oil in shale and insight into the effects of kerogen deformation on flow behavior of oil in shale.

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Generalized Multiscale Approximation of Mixed Finite Elements for Darcy Flow in Fractured Porous Media

Authors: Jie Chen[1]; Zhengkang He[2]; Huangxin Chen[3]

[1] *Xi'an Jiaotong-Liverpool University*

[2] *Xi'an Jiaotong University*

[3] *Xiamen University*

Corresponding Authors: chx@xmu.edu.cn, jie.chen01@xjtlu.edu.cn

We propose a frame work of the mixed generalized multiscale finite element method (GMsFEM) for solving Darcy's law in fractured porous media. The reduced fracture model is adopted for the simulation, where the fractures are modeled by one-dimensional entities. The Raviart-Thomas mixed finite element method is employed for the approximations of the coupled subsurface flows in the matrix and fractures. We approximate matirx pressure in multiscale function space that is between fine-grid space and coarse-grid space. A local cell problem is solved on each coarse-grid element to construct the snapshot space. To construct the multiscale function space of matrix pressure, we further reduce the dimension of the snapshot space by a spectral decomposition. The proposed method for the reduced fracture model preserves the local mass conservation property that is important for subsurface problems. Numerical examples are presented to illustrate the good properties of the proposed approach.

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Microscopic flow mechanism of shale oil based on digital cores with multi-mineral phases

Authors: Lian Duan[1]; Hai Sun[1]; Jun Yao[1]; Lei Zhang[1]; Yongfei Yang[1]

[1] *Research Centre of Multiphase Flow in Porous Media, School of Petroleum Engineering, China University of Petroleum (East China)*

Corresponding Authors: yangyongfei@upc.edu.cn, zhlei84@163.com, sunhaiupc@sina.com, rcogfr_upc@126.com, duanlianupc@163.com

It's important to understand the transport behaviors of fluid through organic/inorganic nanopores for shale oil reservoir development. Flow in nanochannels is affected notably by fluid slippage and adsorption on the nanochannel surfaces. Both slippage and adsorption are related to wettability. The wettability of shale oil reservoir has a wide spectrum from water-wet to mixed-wet and oil-wet due to the multi-mineral phases. In this work, a 3-D digital core with multi-mineral phases is reconstructed from 2-D SEM images of a shale sample. A math model of shale fluid flow considering the slippage boundary condition and varying fluid viscosity is established based on the N-S equation, combined with the slip length formula and apparent viscosity formula obtained by molecular dynamics simulation. Based on the digital core and math model, the single-phase flow simulation is solved based on semi-implicit method for pressure-linked equations (SIMPLE), and the two-phase flow simulation is solved based on volume-of-fluid (VOF) method. By changing the pressure difference and fluid properties, the flow rates in the digital core are obtained, and a relationship chart between the pressure difference and flow rate is made to analyze effects of various factors on the flow.

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Plume deformation, mixing and reaction kinetics in 3-D heterogeneous anisotropic porous media

Authors: Yu Ye[1]; Gabriele Chiogna[2]; Chunhui Lu[1]; Massimo Rolle[3]

[1] *Hohai University*

[2] *Technical University of Munich*

[3] *Technical University of Denmark*

Corresponding Authors: yeyu@hhu.edu.cn, c.lu@hhu.edu.cn, gabriele.chiogna@tum.de, masro@env.dtu.dk

Helical flow can occur in heterogeneous anisotropic porous media where it leads to dilution and reactive mixing enhancement of conservative and reactive plumes. In this study, we performed steady-state flow and transport numerical simulations to investigate helical flow created in three-dimensional porous media and its effect on streamlines deformation, solute dilution and reactive mixing. We considered two macroscopic anisotropic inclusions embedded in a homogeneous porous medium. We constructed 16 different scenarios by changing the geometries and the relative positions of the anisotropic inclusions. Mean flow velocity and metrics of stretching and folding were computed to characterize the flow field, whereas dilution and reactive mixing were quantified using the entropy-based metric of flux-related dilution index and the reactive plume length. Instantaneous and kinetically-controlled reactions were considered in the reactive transport scenarios. The results show that helical flows induce deformation, dilution and reactive mixing enhancement that are dependent on the different helical flow patterns. The extent of streamlines deformation could not be directly related to dilution and mixing enhancement. For reactive transport, we observed significant differences of the reactant dilution when considering different reaction kinetics. The latter resulted in both increasing and decreasing trends of the reactant's entropy. The comparison with analogous simulation in a homogeneous domain showed that the complex 3-D flow patterns, leading to strong mixing enhancement, shifted the system towards a kinetic-limited state in which the contribution of the reactive term and the description of the reaction rates became more important.

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Dynamics of capillary rise and finger formation in angular pores

Authors: Thijs de Goede[1]; Rozeline Wijnhorst[1]; Daniel Bonn[1]; Noushine Shahidzadeh[2]

[1] *University of Amsterdam*

[2] *University of Amsterdam -Institute of Physics*

Corresponding Authors: t.c.degoede@uva.nl, tcdeg1@gmail.com, n.shahidzadeh@uva.nl, d.bonn@uva.nl

The ability of porous materials to absorb liquids with capillary action plays a major role in many industrial and natural processes. Understanding corner flows and their impact on the liquid imbibition dynamics is of paramount importance to fully understand the imbibition processes happening inside complex porous media such as soils, rocks and textiles. Many studies assume that the speed of the

displacement of the main liquid front inside the porous material can be described by Washburn's law, based on spontaneous capillary rise in cylindrical capillaries. However, in real porous media corners and grooves can retain wetting liquids, changing the imbibition dynamics. The wetting phase forms fingers in the corners of angular pores and depending on the structure and wettability, these liquid fingers can extend over macroscopic distances. Consequently, cylindrical capillaries generally are too simple to describe the fluid flow in an irregular porous network.

We present a multiscale study of the dynamics of capillary imbibition in cylindrical and square capillaries as model pores without and with corners. Using high speed camera and fluorescent imaging techniques the capillary rise dynamics and finger formation are measured. The influence of the surface tension of the liquid and gravity on the meniscus rise and the finger formation and growth in the corners of the square capillaries are investigated. We also show how the presence of surfactants modifies the capillary rise and finger formation dynamics by changing the dynamic surface tension. Understanding such corner flows is particularly important for a better understanding and modelling of fluid imbibition in complex porous media such as e.g. paper, textiles that have very elongated and angular pores but also relevant for pollutant transport in soils, that can also take place through corner flows.

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A pore-network model approach for coupling free flow with porous medium flow applied to evaporation

Authors: Kilian Weishaupt[1]; Rainer Helmig[1]

Co-authors: Alex Terzis ; Ioannis Zarikos [2]; Guang Yang [3]; Vahid.J Niasar ; Matthijs de Winter [4]; Dennis Gläser ; Timo Koch

[1] *University of Stuttgart*

[2] *Eindhoven University of Technology*

[3] *Institute of Refrigeration and Cryogenics, Shanghai Jiao Tong University*

[4] *Utrecht University*

Corresponding Authors: rainer.helmig@iws.uni-stuttgart.de, kilian.weishaupt@iws.uni-stuttgart.de, vahid.niasar@manchester.ac.ul dennis.glaeser@iws.uni-stuttgart.de, y_g@sjtu.edu.cn, timo.koch@iws.uni-stuttgart.de, d.a.m.dewinter@uu.nl, i.zarikos@tue.nl

Coupled systems of free flow adjacent to a porous-medium are ubiquitous in nature and in technical applications. Interface-driven transport and exchange processes occur in soil evaporation, fuel cell water management or food drying.

A pore-scale description of these systems (e.g., by means of DNS) is very often unfeasible due to the highly complex geometry of the porous material. Averaged REV-scale approaches may fail to account for pore-scale effects like local saturation distribution patterns in sufficient detail, while those can have a strong impact on the he global behavior of the coupled system.

We propose a novel hybrid model which captures pore-scale effects at the interface in ample detail while still maintaining a comparatively low computational effort. The key feature of this approach is a pore-network model which represents the transition region between the porous matrix and the free flow.

The model comprises three computational domains:
the free-flow region where the (Navier-) Stokes equations are solved, the transition zone described by the pore-network model and a bulk porous domain accounted for by Darcy's law.

Thermodynamic consistency is ensured by appropriate coupling conditions. We follow a monolithic coupling approach such that fluxes of mass, momentum and energy across the domain interfaces are preserved implicitly while no coupling iterations are required. A fully implicit dynamic pore-network model is used in order to resolve flow and transport processes beyond capillary equilibrium. The model is implemented in the open-source porous media simulator *DuMux* which has recently been extend by the capability to couple an arbitrary number of subdomains.

We present a comparison with micro-PIV experimental data for single-phase flow and provide numerical examples of evaporation including non-isothermal, two-phase and two-component flow.

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An investigation into the controls of fracture tortuosity in rock sequences and its impact on fluid flow in the upper crust

Authors: Nathaniel Forbes Inskip[1]; Tomos Phillips[2]; Kevin Bisdom[3]; Georgy Borisochev[2]; Andreas Busch[2]; Sabine den Hartog[2]

[1] *Heriot-Watt*

[2] *Heriot-Watt University*

[3] *Shell Global Solutions International B. V.*

Corresponding Authors: s.den_hartog@hw.ac.uk, tp45@hw.ac.uk, n.forbes_inskip@hw.ac.uk, a.busch@hw.ac.uk, gb168@hw.ac.uk, kevin.bisdom@shell.com

Fractures are ubiquitous in geological sequences, and play an important role in the movement of fluids in the Earth's crust, particularly in fields such as hydrogeology, petroleum geology and volcanology. When predicting or analysing fluid flow, fractures are often simplified as a set of smooth parallel plates. In reality, they exhibit tortuosity on a number of scales: Fine-scale tortuosity, or roughness, is the product of the small-scale (μm –mm) irregularities in the fracture surface, whereas large-scale (> mm) tortuosity occurs as a result of anisotropy and heterogeneity within the host formation that leads to the formation of irregularities in the fracture surfaces. It is important to consider such tortuosity when analysing processes that rely on the movement (or hindrance) of fluids flowing

through fractures in the subsurface. Such processes include fluid injection into granitic plutons for the extraction of heat in Engineered Geothermal Systems, or the injection of CO2 into reservoirs overlain by fine-grained mudrocks acting as low-permeability seals in Carbon Capture and Storage projects.

Although it is generally assumed that tortuosity is controlled by factors such as grain size, mineralogy and fracture mode, a systematic study of how these factors quantitatively affect tortuosity is currently lacking. Furthermore, in anisotropic rocks the fracture orientation with respect to any inherent anisotropy is also likely to affect tortuosity.

In order to address this gap, we have induced fractures in a selection of different rock types (mudrocks, sandstones and carbonates) using the Brazil disk method, and imaged the fracture surfaces using both digital optical microscopy and X-ray Computed Tomography. Using these methods we are able to characterise both the fine-scale (roughness) and large-scale tortuosity. In order to understand the effect of fracture orientation on tortuosity we have also analysed fractures induced at different angles to bedding in samples of a highly anisotropic mudrock taken from South Wales, UK. Results indicate that fine-scale tortuosity is highly dependent on the fracture orientation with regards to the bedding plane, with fractures normal to bedding being rougher than those induced parallel to bedding. Finally, in order to measure the effect of tortuosity on fluid flow, we have carried out a series of core flooding experiments on a subset of fractured samples showing that fracture transmissivity decreases with increasing tortuosity.

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Pore-scale wettability characterization in mixed-wet sandstones using dynamic laboratory micro X-ray tomography

Authors: Arjen Mascini[1]; Marijn Boone[2]; Veerle Cnudde[3]; Tom Bultreys[4]

[1] *University of Gent*

[2] *TESCAN XRE*

[3] *Ghent University, Utrecht Univeristy*

[4] *Ghent University*

Corresponding Authors: tom.bultreys@ugent.be, marijn.boone@tescan.com, arjen.mascini@ugent.be, veerle.cnudde@ugent.be

Multiphase flow is strongly influenced by the wettability of the porous medium. Conventionally, wettability is quantified by the contact angle between the fluid-fluid interface and the solid surface. Recent attempts to measure contact angles directly (AlRatrout et al., 2017; Scanziani et al., 2017) and indirectly (Blunt et al., 2019) from micro X-ray tomographic images have proven to be challenging due to the scale-dependent and hysteretic nature of contact angles. In principle, the contact angle that controls the invasion process has to be measured at (or at least near) the moment the fluid interface moves into a neighboring pore. Laboratory based dynamic micro X-ray tomography (Bultreys et al., 2016) offers the possibility to perform challenging experiments in a controlled laboratory environment, with acquisition times and image quality close to those achieved at synchrotron facilities. For this study, n-decane-brine drainage and imbibition experiments were performed on two medium-grained calcareous sandstone samples from the Luxembourg Sandstone Formation (lower Jurassic). One of these samples was treated using octadecyltrichlorosilane (OTS) to induce an intermediate to mixed wettability distribution. The experiments were imaged continuously using a laboratory based micro X-ray tomography scanner optimized for fast image acquisition to generate a time series of micro-CT images. For each image, pore-scale properties such as fluid distributions, fluid-fluid interfacial curvatures and contact angles were calculated. Using a clustering algorithm, neighboring pores that change fluid occupancy are clustered together allowing calculations of pore-scale properties on an event-by-event basis. Measurements of the pore scale properties are validated by performing

high resolution region of interest scans (2um/voxel) at the end of drainage and imbibition. By combining image-based pore-scale properties with spatial connectivity information, wettability can be characterized at the pore-scale to inform numerical simulations of multiphase flow.

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Electrolyte Transport through the Porous Electrode in Vanadium Redox Flow Batteries

Authors: Nico Bevilacqua[1]; László Eifert[1]; Kerstin Köble[1]; Rupak Banerjee[2]; Tomas Farago[1]; Marcus Zuber[1]; Aimy Bazylak[3]; Roswitha Zeis[1]

[1] *Karlsruhe Institute of Technology*

[2] *Karlsruhe Institute of Technology*

[3] *University of Toronto*

Corresponding Authors: marcus.zuber@kit.edu, rban86@gmail.com, kerstin.koeble@uni-ulm.de, tomas.farago@kit.edu, laszlo.eifert@kit.edu, nico.bevilacqua@kit.edu, abazylak@mie.utoronto.ca, roswitha.zeis@kit.edu

With a continuous growth in the contribution of renewable energy sources to the electricity grid, grid-scale energy storage has become an area of considerable interest. Redox flow batteries allow the decoupling of energy and power capacity, allowing for large scale storage opportunities [1,2]. It has been estimated by the United States Department of Energy that a cost of 120 $/kWh would make the technology viable for grid-scale storage deployment [3]. Cost of components and the electrolyte play a key role in reducing the cost of redox flow batteries.

Porous carbon felt materials have been found to be the most suitable as electrode materials for Vanadium Redox Flow Batteries (VRFBs) [4]. These porous materials provide the surface area for the electrolytes on both the positive and negative half cells to react and participate in the energy exchange. The SGL Group produces commercially available carbon felt products for this purpose. In this work, selected materials from the SGL Group were evaluated for their transport properties with regard to electrolyte flow in VRFBs. Therefore, in-situ synchrotron x-ray radiography and tomography experiments have been conducted, whereby the electrolyte was injected into the flow cell using a peristaltic pump [5]. The flow of the electrolyte through the porous electrode was tracked during the injection process via radiography images. Simultaneously, the pressure drop was measured to characterize the transport process and identify the breakthrough of the electrolyte on the opposite side of the electrode. These measurements informed our theoretical models to better understand the multiphase and interfacial flow phenomena within the porous electrode, which is essential for the evaluation and optimization of electrode materials currently being used in VRFBs.

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An Efficient Parameterization for History Matching of Reservoir Models by Using Deep Variational Autoencoder with The Intrinsic Dimension Estimation Method

Authors: Xiaopeng Ma[1]; Kai Zhang[2]

[1] *China university of petroleum (east China)*

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

Corresponding Authors: xiaopeng.ma.cn@gmail.com, zhangkai@upc.edu.cn

Efficient parameterization of spatially distributed grid variables such as permeability, porosity, etc. is essential for automatic history matching of complex geological reservoirs. While the initial prior ensemble of reservoir models can be established using geostatistical modeling methods using data from seismic, borehole logs, core, and other technologies, the low-dimensional parameterized representation of the reservoir model can be learned by machine learning methods. Recently the success of deep generative models in matching learning communities has encouraged an intense research activity to develop various parameterizations methods for complex reservoirs. In this study, intrinsic dimension estimation is introduced into the deep variational autoencoder model to allow us to learn the low-dimensional representation efficiently. Specifically, we employ the singular value decomposition and propose a new intrinsic dimension estimation method according to the singular value difference spectrum to estimate the intrinsic dimension of the reservoir model parameter, which is robust for large datasets. The proposed parameterization method was combined with the ensemble smoother with multiple data assimilation and tested in history matching of three synthetic channelized reservoirs. The experiments showed promising results, outperforming previous methods and generating well-defined posterior channelized facies.

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Combined effects of network topology, hydraulic conditions and in-situ stress variations on solute propagation in natural fracture networks

Authors: Chuanyin Jiang[1]; Xiaoguang Wang[2]; Delphine Roubinet[3]; Zhixue Sun[1]

[1] *China University of Petroleum - East China*

[2] *Hydrosciences Montpellier*

[3] *Geosciences Montpellier-CNRS, University of Montpellier*

Corresponding Authors: delphine.roubinet@umontpellier.fr, x.wang0127@gmail.com

Fractured rocks are involved in a large range of environmental applications for which the topological properties of the fracture network are determinant. In general, these structures represent quick and localized main paths which interact with the surrounding low-permeability matrix. For the propagation of tracer and contaminant, the strong contrast in geometrical and physical properties between the fractures and matrix, and the heterogeneities inherent to each domain, imply that (i) standard solving methods (finite volume, finite element$\cdots$) are not adapted to solve the corresponding advection-diffusion and advection-dispersion equations, and (ii) these systems are characterized by anomalous behaviors that cannot be upscaled with standard multi-continuum approaches.
In this work, we consider the natural fracture pattern of Triassic limestone exposed at the southern margin of the Bristol Channel Basin in United Kingdom for which we perform multi-directional solute transport simulations under various hydraulic conditions and in-situ stress configurations. We analyze under which conditions (i) these simulations require the use of particle-based methods, (ii) the surrounding matrix has a determinant impact of the resulting breakthrough curves, and (iii) the upscaling of the corresponding transport processes is feasible with various techniques, going from standard multi-region to Markov-directed random walk methods.
From these simulations, we analyze the impact of the considered flow direction in order to gain indications on the characterization of hierarchical natural joint networks. We also evaluate how the contrast in the topological properties of the considered fracture sets and the stress-dependent aperture distributions play a role in the spatial properties of the flow paths and particle trajectories. These results enrich our understanding of the complex interplay between fracture network topology, hydraulic boundary and in-situ stress, and of their impact on flow and transport properties.

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Pore-Scale Modeling for Open-Sorption Pipe Reactor by Lattice Boltzmann Method

Authors: Bin Guo[1]; Huijin Xu[1]; Changying Zhao[1]

[1] *Shanghai Jiao Tong University*

Corresponding Authors: xuhuijin@sjtu.edu.cn, guobin0615@sjtu.edu.cn, changying.zhao@sjtu.edu.cn

urrently, considerable researches about sensible and latent heat storage have been conducted and various reactors have been designed and developed, while the process and reactor of thermochemical heat storage, with higher energy density and longer heat storage period, still need further study. In this paper, we concentrate on a novel type of open-sorption pipe reactor and attempt to reveal the thermochemical reaction mechanisms inside on pore scale mainly through Lattice Boltzmann Method. The heat storage reactor being studied consists of sorption pipe units with a perforated diffuser pipe network and the thermochemical heat storage material (calcium oxide) filled in between,

which reacts with water entering from the inlet, so that heat can be stored through the chemical reaction. Thus, numerical models with different porosities, hole sizes and hole distances are established, besides, parameters related to flow, reaction and other influence factors are studied and compared with each other in order to obtain optimal results. As a result, this new type of reactor performs better than the direct mixing tube reactor and the number of holes on diffuser pipe have a significant impact on the material concentration of the outlet. The conclusions of the paper possibly play a positive role on heat storage system design.

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The influence of microfractures on hydrocarbon migration

Author: Wenqing Tang[1]

Co-authors: Taixun Liu [2]; Xiangying Wang ; Jin Wang [3]; Ping Wang [2]

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

[2] *China University Of Petroleum*

[3] *China University of Petroleum*

Corresponding Authors: 1404195190@qq.com, 846396194@qq.com, 695975871@qq.com, 1357935524@qq.com, 478684961@qq.com

Fractures play an important role in migration and accumulation of hydrocarbon and permeability of reservoirs. In this paper, the coherent body, variance body, ant body and dip-angle lighting techniques are used to identify and explain fractures, the characteristics of fracture system and structural style are analyzed, and combined with regional structural background and stress characteristics, analyze the causes of the fractures in the study area, and evaluate the sealing and sealing characteristics of the main faults. The model of fault and stratum is established, and the effect of fractures on hydrocarbon seepage is studied through numerical simulation. The migration path and direction of hydrocarbon are determined. Small micro faults derived from regional stress mainly develop in this area, including small micro faults formed at the end of faults and small micro faults formed at the bending part of faults. When hydrocarbon is transported through the fault structure, step-like migration and one-way vertical migration are inseparable from the role of faults. The fault site serves as a migration channel for hydrocarbon, allowing hydrocarbon to migrate in an orderly manner. The existence of fracture can obviously improve the permeability of reservoir, and the influence of connectivity fracture is more obvious. Through the role of fracture, the path of hydrocarbon migration can be changed, and the blockage of oil and gas migration path can be reduced.
Key words: fracture; fracture system; hydrocarbon migration; numerical simulation

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Multiphysics modeling of a vanadium redox flow battery

Authors: Vanesa Muñoz Perales[1]; Santiago Enrique Ibañez-León[2]; Sabrina Berling[3]; Enrique García-Quismondo[3]; Jesús Palma[3]; Pablo Ángel García-Salaberri[2]; Marcos Vera[2]

[1] *University Carlos III de Madrid*

[2] *Universidad Carlos III de Madrid*

[3] *Instituto IMDEA Energía*

Corresponding Authors: mvera@ing.uc3m.es, enrique.garcia@imdea.org, vamunozp@ing.uc3m.es, sibanez@ing.uc3m.es, jesus.palma@imdea.org, sabrina.berling@imdea.org, pagsalab@ing.uc3m.es

Porous electrodes are an essential component of Vanadium Redox Flow Batteries (VRFBs), which are one of the most relevant technologies among energy storage systems, crucial for the integration of renewable energies into the electrical system. Multi-physics modelling of electrochemical devices is an indispensable tool for the optimization of VRFB performance [1-6].

In this work, a two-dimensional, macroscopic, isothermal, steady-state model of a VRFB is presented. The model accounts for a comprehensive description of charge and mass transport of ionic species and electrochemical kinetics in the porous electrodes. Diffusion and migration are incorporated in the species transport equations, as well as species crossover across the membrane. The properties of the electrolyte (viscosity, density and ionic conductivity) are characterized as a function of the State of Charge (SOC) based on experimental data, thus, providing a more accurate description of species transport.

The model enables an extensive understanding of the coupled phenomena that take place in VRFBs, including the influence of electrode thickness, and electrolyte properties on the charge-transfer current density and the ionic conductivity. Besides, the model can be used to predict the behaviour and performance of the system under different operating conditions and to identify those parameters that are critical for the optimization of the cell design. Several parametric studies are performed to analyse the influence of operating conditions in the polarization curve, open circuit voltage (OCV), and charge and discharge curves. The effect of reaction kinetics, flow rate and SOC on activation and polarization losses is also examined.

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Experimental investigation of contact angle change and oil globule movement in a capillary

Author: Lifei Yan[1]

Co-authors: Hamed Aslannejad [1]; S. Majid Hassanizadeh [1]; Amir Raoof [1]

[1] *Utrecht University*

Corresponding Author: l.yan@uu.nl

Numerous experimental observations and field applications have confirmed that low-salinity water flooding is an effective technique for enhanced oil recovery. Given the involved complex physical and chemical processes, several controlling mechanisms have been proposed to explain the oil release from the rock pores due to low-salinity effects. Osmosis and water-in-oil emulsification are among these mechanisms. However, because of the complexity of brine-oil-rock interactions, our knowledge of these processes is limited and their associated time scales are not well understood.
In this paper, to study the potential contributions of these two factors, experiments using 11 capillary tubes with an inner diameter of 800 μm are used to inject a sequence of low-salinity water, crude oil, and high-salinity water phases and to observe the evolution of the system. The monitoring was done for a period of 40 days. We used two setups, based on imaging using a CMOS camera and a confocal laser scanning microscopy, to dynamically capture the remobilization of oil globule and to measure the 2D/3D contact interfaces, respectively. Next to these image-based observations, microscopic pore pressures were directly measured at both low and high-salinity water phases containing the oil globule. This was done using two microscopic fiber-optic sensors inserted into the capillary. We observed that in the water-wet capillaries the oil globule moved a distance of about 524 μm. The contact angles at both low and high-salinity water interfaces with crude oil gradually decreased by 34.32° and 18.23°, respectively, during the first 15 days. We found that the pressure difference between high/low-salinity water phases reached a plateau with a maximum value of 1.65kPa after a period of 24 days, which is explained with using the observed contact angle changes. Further, we have discussed the basics of osmotic pressure and water diffusion in the crude oil phase.

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The Impact of Grid Refinement on Simulated Injectivity in Surfactant-Alternating-Gas Foam Enhanced Oil Recovery

Authors: Rodrigo Orlando Salazar Castillo[1]; Lily Qian[2]; William R. Rossen[3]

[1] *TU Delft now at Mexican Institute of Petroleum*

[2] *TU Delft now at Kosmos Energy LLC*

[3] *TU Delft*

Corresponding Authors: w.r.rossen@tudelft.nl, lilyqian3808@gmail.com, rosalazar@imp.mx

Surfactant-alternating-gas (SAG) is the primary means of injection of foam for enhanced oil recovery. Recent studies show that conventional simulation cannot accurately simulate injectivity in SAG without extraordinary grid refinement (1). We examine the effect of a series of grid refinements on calculated pressure rise at an injection well for SAG process, based on simulation parameters fit to laboratory data, to show how accuracy improves with grid resolution. We also apply fractional-flow theory (with effectively infinite grid resolutions) to determine if the foam model itself is capable of reproducing the complex behavior of foam near the wellbore reported recently by Gong et al. (2).
We employ a widely used commercial foam simulator, the CMG simulator STARS. We fit the foam parameters to a scan of foam behavior as a function of injected gas fraction. We apply the Peaceman equation (3) to simulate gas and liquid injection in a SAG process in a homogeneous reservoir comprising a 5x5 array of square grid blocks of length L=20 m. Then we subdivide the central grid block itself into a 3x3 array, and then into a 5x5 array, always with the injection well in the center of the central grid block. We compare the pressure rise at the injection well to grid-block pressures further from the well. We also construct the fractional-flow solutions for the injection of gas following the injection of surfactant and for the injection of liquid following the injection of gas.
As shown by Leeftink et al. (4), there is a long-lasting, erroneous, large pressure rise at the injection well in the simulation because the Peaceman equation does not resolve shock fronts or variations of saturation and mobility very near an injection well, which are critical to foam injectivity in SAG. The magnitude of the error decreases as the grid is refined. The duration of the error drops more quickly as L2. Injectivity remains poor indefinitely, however, depending on foam parameters, if the foam model does not account for foam collapse under dry conditions near the well. Similar results obtain for liquid injection.
There are two challenges to accurate simulation of foam injectivity: failure to include crucial mechanisms in the simulator model (2), and the need for extraordinary grid refinement. This study shows that even if the description of the foam model is accurate, corrections (e.g., negative skin factor) are necessary in the absence of extraordinary grid refinement, especially shortly after slug injection is switched between liquid and gas.

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Simulating vertebroplasty: A look into the biomechanics and modelling challenges

Authors: Zubin Trivedi[1]; Christian Bleiler[1]; Arndt Wagner[1]; Oliver Röhrle[1]

[1] *University of Stuttgart*

Corresponding Authors: roehrle@simtech.uni-stuttgart.de, zubin.trivedi@imsb.uni-stuttgart.de, christian.bleiler@imsb.uni-stuttgart.de, arndt.wagner@mechbau.uni-stuttgart.de

Vertebroplasty is a medical procedure done on weakened or damaged vertebral bones to restore their load-bearing capacity. In this procedure, a cement-like polymer (bone cement) is injected percutaneously into the porous trabecular structure inside a vertebral bone, and left for curing. Although the procedure offers a good success rate, there are some risks involved in the clinical application, e.g. leakage of the bone cement could lead to problems like pulmonary embolism or paralysis. To mitigate such a risk, modelling and simulating the procedure, especially the spreading of bone cement upon injection, could be typically useful. The in-vivo system, like all biological systems, entails elaborate biomechanical phenomena. These phenomena include the curing of bone cement during injection, the presence of bone marrow, deformations of the trabecular bone, and subject-specific variation. This contribution investigates different biomechanical aspects and related hurdles in modelling, e.g. the complex behaviour of the biomaterials, while exploring ways to navigate around them.

A macroscopic continuum-mechanical framework using the Theory of Porous Media (TPM) serves as the main platform for the presented multiphasic model; consisting of bone, bone marrow, and bone cement. This is built upon using realistic constitutive models, e.g. time-dependent viscosity of the bone cement, capillary pressure-saturation relations, etc. Furthermore, pore-scale simulations, viz. CFD simulations using finite elements and Fluid-Structure-Interaction simulations, are carried out to incorporate geometry and interface effects at the macro-scale via upscaling. Apart from this, parametric studies using pore-scale simulations on regular microstructures are implemented to identify the important geometric parameters on the macro-scale. The validation of the model is studied using an experimental setup that injects bone cement into structures similar to the trabecular bone, while being imaged through dynamic CT. Finally, potential ways forward to improve vertebroplasty are explored and discussed.

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Utilization of microporous materials as multi-functional proppant for enhanced shale gas and recovery and CO2 sequestration

Authors: Kaiyi Zhang[None]; Guan Qin[1]

[1] *University of Houston*

Corresponding Authors: gqin2@central.uh.edu, kzhang11@uh.edu

The ever-growing global energy demand and the urge to reduce greenhouse gas emissions is driving us toward cleaner energy resources, higher recovery factors and techniques for carbon sequestrations. Thus, we propose a novel approach to use microporous materials such as zeolites as multi-functional proppants to enhance shale gas and oil recovery and sequestrate CO2 geologically.
The idea behind this approach is that, by careful selection of the target materials, the microporous materials or the multi-functional proppants can adsorb large quantities of CO2 and be delivered into shale reservoirs through hydraulic fracturing stimulations. The adsorbed CO2 is then released from the proppants and preferentially adsorbed by shale organic matter at reservoir condition. In such a way, sorbed gas can be replaced by CO2 and CO2 can be sequestrated. This approach can also be extended to enhanced oil recovery for broader application.
To validate the thermodynamic feasibility of these processes, we conduct Grand Canonical Monte Carlo (GCMC) simulation to examine the adsorption properties of our target material and the shale

organic matter. We first simulate competitive adsorption of CH4 and CO2 in silicalite-1, a characteristic all-silica zeolite framework and kerogen organic matter and compare the adsorption selectivity of CO2 over CH4 in those materials. The adsorption isotherms show that both silicalite-1 and kerogen have stronger preference of adsorbing CO2 over CH4 under most conditions and kerogen always has a higher CO2/CH4 selectivity than silicalite-1 does. These findings ensure a net flow of CO2 from the zeolites to the kerogen organic matter and there will be no excessive adsorption of CH4 by silicalite-1.
Then we extend our work to systems with water present. Since water is the major component and the carrier to deliver the CO2-loaded proppants into shale reservoir during a hydraulic fracturing stimulation, it is of our primary interest to investigate the impact of water on the adsorption properties of CO2 and CH4 in shale organic matter and in zeolites. We construct systems of CO2 and CH4 with different water contents and compare the results with the non-water cases. It is found that water can significantly alter the CO2/CH4 selectivity of silicalite and kerogen under some circumstances, but the kerogen is still more CO2-selective than silicalite.
The results from our GCMC simulations validate the thermodynamic feasibility of using zeolites as multi-functional proppants that carry CO2 to shale reservoirs for enhanced shale gas recovery an CO2 sequestration. Our future work focuses on the application in shale oil reservoirs, the screening of the target materials and the simulation of the dynamic process of adsorption/desorption and proppant transport.

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"Hot Spots"observed in pore scale simulation of flow in carbon fibre felt electrodes may limit the efficiency of Redox Flow Battery operation

Authors: Farrel Gray[1]; IOANNIS ZACHAROUDIOU[1]; Rhodri Jervis[2]; Edo Boek[3]

[1] *Imperial College London*

[2] *University College London*

[3] *Queen Mary University of London*

Corresponding Authors: e.boek@qmul.ac.uk, farrel.gray@imperial.ac.uk, rhodri.jervis@ucl.ac.uk, i.zacharoudiou@imperial.ac.uk

The Vanadium Redox Flow Battery (VRFB) is one of the most promising Electro-Chemical Device (ECD) technologies for large scale local storage of renewable energy, such as wind and solar. Commercial exploitation of this technology has emerged, but a lack of fundamental understanding regarding VRFB operation is limiting the development of this new technology. In particular, the energy density must be improved. For this reason, we investigate here the performance of carbon fibre electrode materials using a combination of computational modelling and experimental characterisation. In particular, the surface area of the porous electrode is critical to the device performance. To optimize electrochemical reactions in the electrode, the reactive surface area has to be as large as possible. In terms of micro-structure, this means that the felt fibres must be distributed homogeneously. In current VRFB technology, however, the felts are woven bundles of fibres yielding a large local variation in voids and bundles. Recently, synchrotron micro-CT scanning was used [A] to image the 3D pore structure of a graphite felt in-operando. However, the resulting alteration of the actual flow field could not be quantified, as it is very difficult to measure in-situ due to limited spatio-temporal resolution. Also, it is difficult to obtain the altered flow field from average tortuosity and porosity calculations, as the relation between permeability and tortuosity / porosity is only known empirically. Here we calculate the relation between flow and altered micro-structural properties using direct flow calculations in pore space images of a representative volume of a carbon fibre material obtained from micro-CT imaging. In Figure 1 we present a 3D fibre felt geometry, obtained from micro-CT experiments, and the corresponding flow field, as a test for large volume calculations.

The flow field was calculated using our home-grown Lattice-Boltzmann (LB) code (see [D]) on a big data set of 15 billion voxels using HPC facilities.

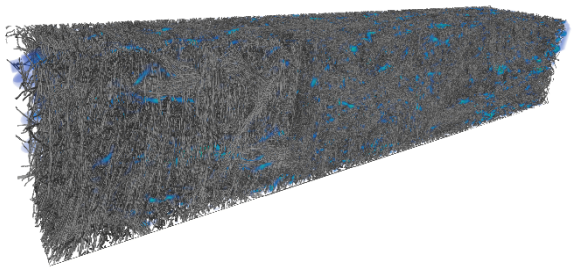

Figure 1: Micro-CT pore space image of carbon fibre felt combined with single phase LB calculations of the flow field. Blue colour indicates "hot spots"in the flow field

From this figure, we observe that the electrolyte is concentrated in local areas ("hot spots"), thus limiting electrochemical reactions. The heterogeneity of the commercial soft carbon fibre material therefore may reduce the efficiency of the electrode, as it may cause high voltage spots and therefore damage in the electrode. In addition, under certain electro-chemical conditions, H2 and O2 gas bubbles may develop in the pore space of the heterogeneous electrode, associated with detrimental effects on VRFB performance [A]. Therefore we extend our multi-phase LB code to investigate the development of gas bubbles in the electrode (Fig.2), initially by seeding random gas bubbles, based on our previous work on multi-phase flow in natural porous materials [B,C]. To mitigate problems associated with the heterogeneous nature of carbon fibre graphite felts, we propose a rational design approach to develop new carbon materials with superior properties.

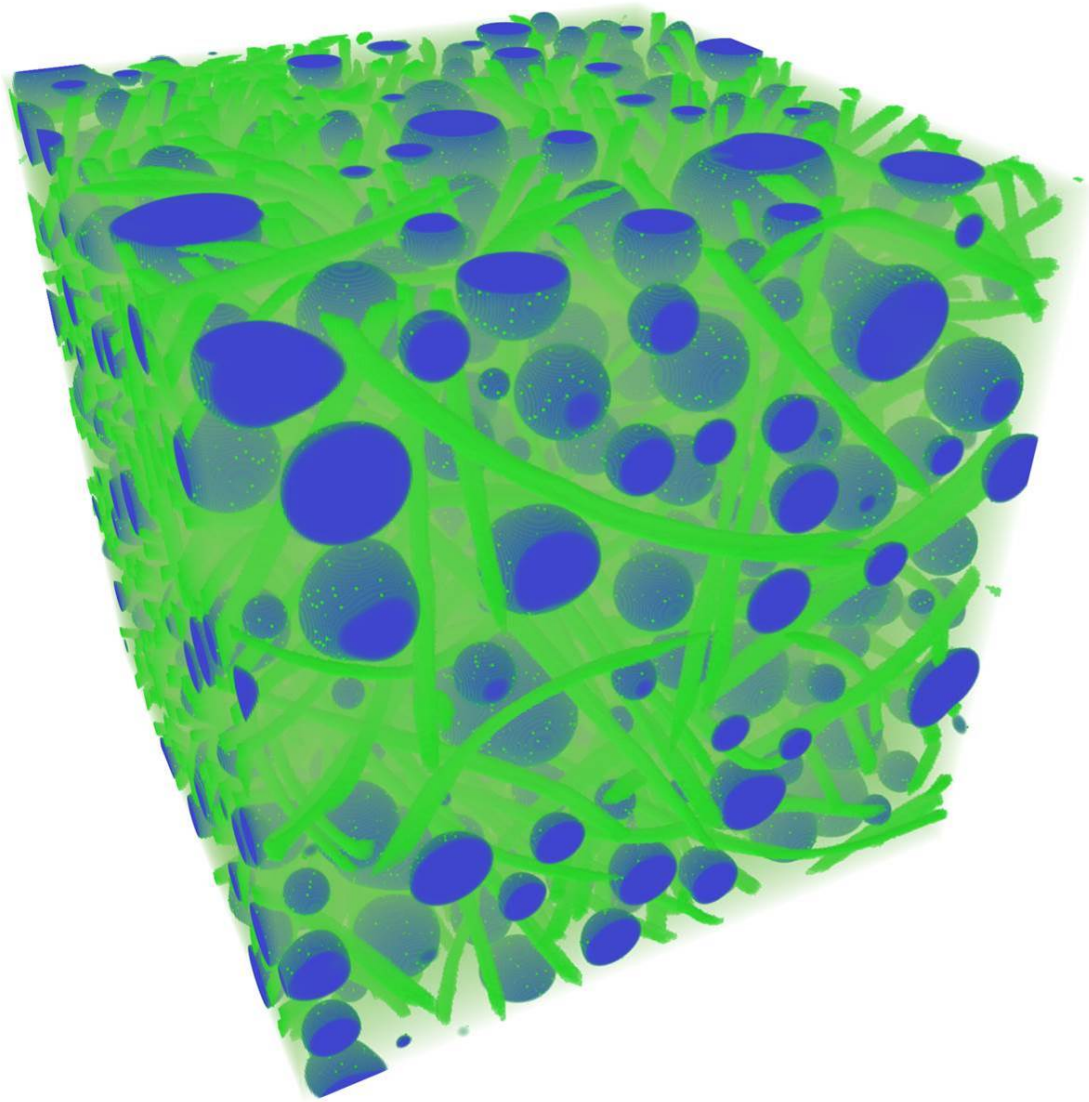

Figure 2: Multi-phase gas-liquid LB calculation of development of gas bubbles (blue) in carbon fibre (green) electrode.

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Visualization of Polymer Retention Mechanisms in Porous Media using Microfluidics

Author: Antonia Sugar[1]

Co-authors: Serag F. Maged [1]; Victor A. Torrealba [2]; Ulrich Buttner [1]; Satoshi Habuchi [1]; Hussein Hoteit [1]

[1] *KAUST*

[2] *Chevron Corps*

Corresponding Author: antonia.sugar@kaust.edu.sa

Understanding polymer transport through porous media is key to successful field implementations including well conformance control and EOR processes. Polymer retention is typically assessed indirectly through their effect on pressure drops and effluent concentrations. Microfluidic techniques represent optimal tools to observe and quantify polymer retention in porous media. In this paper, we demonstrate, how a soft-lithography microfluidics protocol can be used to gain insights into polymer transport mechanisms through rocks.

The design of the microfluidic chips honors the pore-size distribution of oil-bearing conventional reservoir rocks, with pore-throats ranging from 2 to 10 μm. The current fabrication techniques enabled us to transfer the design on a silicon wafer substrate, through photolithography. The etched wafer holding the negative pattern of the pore-network served as mold for building the microfluidics chip body out of polydimethylsiloxane (PDMS). The oxygen plasma bonding of the PDMS part to a thin glass slide resulted in a complete microfluidic chip, conceptually referred as "Reservoir-on-a-Chip". Microfluidic chips serve as a two-dimensional proxy, where we remove the inherent complexity of the three-dimensional porous network in rocks, which facilitate narrowing into the mechanisms that occur at pore-scale. Hence, we conduct single-phase polymer flooding experiments on the designed chips to study their transport behavior. These experiments allowed us to visualize polymer transport at the molecular scale owing to the use of polymer tagging and super-resolution imaging techniques.

The paper presents a direct visualization of polymer retention mechanisms in porous media, for the first time. We identified three mechanisms leading to polymer retention: adsorption, mechanical entrapment, and hydrodynamic retention. Polymer adsorption on the chip surfaces resulted in flow conductivity reduction in specific pathways and complete blockage in others, and generated changes in the flowpaths. This mechanism occurred almost instantaneously during the first minutes of flow then dramatically diminished as adsorption was satisfied. In addition to this static adsorption, flow-induced adsorption (entrapment) was also distinguished from binding of flowing polymer molecules to the already adsorbed polymer layer. Evidence of polymer desorption was observed, which consents with the presumed reversibility character of polymer adsorption mechanism. The narrowest channels along with the reduced area due to adsorption, created favorable conditions for polymer entrapment. Both mechanical and hydrodynamic trapped polymers were captured. These phenomena led to polymer clogging of porous network, which was identified to be one of the major concerns for operational aspects of polymer flooding processes. The particle tracking velocimetry analysis of various injection flow-rate scenarious (7 μl/min, 5 μl/min, 3μl/min, 1 μl/min and even lower) resulted in velocities between 3 and 23 ft/day; values which are representatives for field conditions.

Better understanding and quantification of polymer retention in porous media can help make better decisions related to field-scale implementations of polymer-based processes in the subsurface. In this study, we used a soft-lithography fabrication technique and super-resolution microscopy, to show for the first time polymer transport insights at the pore-scale.

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Preliminary Study on Mechanical Model of Reef Limestone Porous Media

Authors: Ning Zhang[1]; Cijia Wang[1]; Thomas Nagel[2]

[1] *Nanjing University of Science and Technology*

[2] *Technische Universität Bergakademie Freiberg*

Corresponding Authors: zhangning@njust.edu.cn, thomas.nagel@ifgt.tu-freiberg.de

Natural reefs are formed by coral sedimentation and petrification near coasts in tropical regions. Very little is know the deformation behaviour and the structural evolution of the reefs under the impaction of the ocean wave. To investigate these aspects further, we extracted reef limestone samples from the reef(Fig. 1) located at Xisha Islands. Fig. 1 shows the remarkable pore characteristics of a reef limestone sample. Based on preliminary testing of the basic mechanical properties of reef limestone [3,4], this paper intends to construct a $p-\alpha$ constitutive model to describe the equation of states of reef limestone under dynamic loading 2, the typical $p-\alpha$ model gives a good representation over the entire stress range, since many problems involve both high and low stresses at different times and positions in the motion 1. The model has been tested in a dynamic finite element analysis.

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Fig.1 Reef limestone sample

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Pore-network modeling of gas diffusion layers in polymer electrolyte fuel cells using a continuum-based formulation

Authors: Pablo Ángel García-Salaberri[1]; Iryna Zenyuk[2]; Jeff Gostick[3]; Adam Z. Weber[4]

[1] *Universidad Carlos III de Madrid*

[2] *Tufts University*

[3] *University of Waterloo*

[4] *Lawrence Berkeley National Laboratory*

Corresponding Authors: azweber@lbl.gov, pagsalab@ing.uc3m.es, iryna.zenyuk@tufts.edu, jgostick@uwaterloo.ca

A pore-network formulation is presented to model gas diffusion layers (GDLs) in polymer electrolyte fuel cells (PEFCs) using a continuum-based approach. The formulation can easily be integrated into macroscopic models in CFD codes, thus improving the modeling predictions while keeping a moderate computational cost.

The continuum-based pore-network formulation is based on a cubic lattice 1, which is divided into control volumes (cubes) of prescribed size. Pores and throats are placed inside the control volumes, and "connectors"of negligible volume interconnect the control volumes. The "connectors"are used to regulate the invasion-percolation pattern according to the size of the throat that links the pores within neighboring control volumes. Hence, the formulation can account for both invasion-percolation between pores as well as evaporation/condensation in the pore volume inside each control volume. 27 computational cells are used to mesh each control volume. This is a major advantage compared to traditional pore-network models based on a fully discrete formulation where phase-change phenomena are difficult to implement. Local anisotropic effective transport properties (permeability and diffusivity) are determined using a 1D resistor network analogy inside each control volume according to the size of the pore and throats in it.

The model is validated against capillary pressure curves and effective transport properties (effective diffusivity and permeability) measured ex situ. In addition, water saturation profiles are compared with distributions obtained using X-ray computed tomography.

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A fully coupled Thermo-Hydro-Chemo-Mechanical model for the evaluation of gas production characteristic in hydrate-bearing sediment

Author: Didi Wu[1]

Co-author: Shuxia Li [1]

[1] *School of Petroleum Engineering, China University of Petroleum*

Corresponding Authors: lishuxia@upc.edu.cn, b16020087@s.upc.edu.cn

Hydrate decomposition kinetics, multi-phase flow, heat transfer and deformation are significant mechanisms in gas hydrate reservoirs. However, stress dependence of matrix pores does not draw as much attention in numerical simulators. Moreover, all these effects interact with each other closely, which can lead to additional complexity of gas transport and production. Therefore, development of an integrative model with consideration of these complicated mechanisms is needed. In this paper, we develop such a fully coupled model for gas hydrate reservoir simulations. The Darcy flow is corrected by using threshold pressure gradient, which is reasonable especially in the case of high hydrate saturation. In particular, a fully two-way coupling model is developed based on the solution platform of finite element method. Numerical simulations are performed in both core-scale and field-scale cases and compared with experimental data and trial production data from Nankai Trough in Japan. The simulations indicate that the new simulator lead to consistent production characteristic. By use of this validated simulator, the effects of the model parameters upon the hydrate dissociation, gas transport and production are studied, and a variety of new insights are achieved by applications with respect to real hydrate reservoirs.

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The influence of confining pressure and flow process on the corrosion of wellbore cement under geological storage environment

Author: Manguang Gan[1]

Co-authors: Liwei Zhang [1]; Xiuxiu Miao [1]; Yan Wang [1]; Xiaochun Li [1]

[1] *State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences*

Corresponding Authors: cumtgmg@163.com, zlw_85@foxmail.com

One of the major technological issues for CO2 geologic sequestration is the long-term behavior of the wellbore cement used to ensure the overall sealing performance of the storage wells. Thus, understanding CO2-rich brine induced changes to the imperfections in cement matrix is vital for predicting whether CO2 would leak or not. In order to explore the effect of confining pressure and flow process on the corrosion of wellbore cement and development of leakage channel in wellbore cement under the condition of CO2 geological storage, we carried out comparative experiments of which CO2-saturated brine flow through cement sample and no flow case under different confining pressure, and then used micro-computed Tomography (CT) scanner and scanning electron microscope (SEM) on the experimental samples to study the structural changes and used X-ray diffraction (XRD) and inductively coupled plasma mass spectrometry(ICP-MS) to detected the changes of the chemical composition of cement samples. In the no flow experiment, we selected 17 MPa or 20 MPa confining pressure and 17 MPa pore pressure to study the influence of confining pressure on the process of cement corrosion. In the flow experiment, we selected 0.01 ml/min and 0.1 ml/min as the flow rate in the condition of 20 MPa confining pressure and 17 MPa pore pressure. Findings from this work will provide valuable insights applicable to figure out how wellbore cement corrosion in different confining pressure and CO2 injection rate in in-situ CO2 geological storage environment.

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Numerical Modeling of Wettability Alteration in Porous Media Induced by Low Salinity Water

Authors: Takashi Akai[1]; Martin Blunt[1]; Branko Bijeljic[2]

[1] *Imperial College London*

[2] *Imperial College*

Corresponding Authors: b.bijeljic@imperial.ac.uk, t.akai17@imperial.ac.uk, m.blunt@imperial.ac.uk

Low salinity water flooding (LSWF) is a method for crude oil extraction from subsurface reservoirs, in which water whose salinity is lower than that of formation brine is used to improve oil recovery. LSWF generates much interest in oil industries as an economical and environmentally-friendly improved oil recovery method. The most accepted underlying mechanism in the literature is wettability alteration toward more water-wet states caused by the thickening of thin water films covering rock surface with a thickness of typically less than 10 nm.

In this work, we present the numerical modeling of wettability alteration induced by LSWF at the pore-scale. We examine how wettability alteration at the rock surface results in additional oil recovery in the complex 3D pore space of rocks.

Two transport equations were solved with the lattice Boltzmann (LB) method: the Navier-Stokes equation for immiscible two-phase oil and water flow and the advection-diffusion equation for the transport of ions in water. Crucially, we developed a wettability alteration model which mimics the effect of wettability alteration occurring in a water film which is below the resolution of the simulation model. The kinetics of wettability alteration in our model is controlled by two parameters representing the sensitivity of the wettability alteration to water salinity and the rate of the alteration.

Our numerical model was first validated against published experiments where wettability alteration by low salinity water was observed in simple and regular pore geometries. Then, the model was used to simulate LSWF in a complex 3D pore structure of a rock sample obtained with 3D X-ray micro-CT. We observed that residual oil after high salinity water flooding was, at first, remobilized by wettability alteration induced by low salinity water, and then it became connected with the surrounding oil. As a result, higher oil recovery was obtained, compared to high salinity water flooding. Moreover, our parametric study on injection schemes and parameters in the wettability alteration model revealed that the difference in the mixing state between injected low salinity water and high salinity water originally present in the pore space resulted in different oil recoveries.

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Flue Gas Hydrate Storage, Self-Preservation and Dissociation in Unconsolidated Porous Medium in the Presence of Environment-Friendly Promoters

Author: Jyoti Shanker Pandey[1]

Co-author: Nicolas von Solms [1]

[1] *Technical University of Denmark*

Corresponding Authors: nvs@kt.dtu.dk, jyshp@kt.dtu.dk

Gas storage, such as carbon storage in the geological setting, is seen as a useful technique to mitigate the impact of climate change. When Flue gas containing different CO2 mole % is injected into sediments, at a specific pressure and temperature range, CO2 hydrate can be formed as a by-product, which could act as a seal against the possible leaking of CO2 over an extended period. CO2 hydrate formation can be accelerated in the presence of certain chemicals known as hydrate promoters. Effect of these promoters on hydrate self-preservation tendency and dissociation behavior is also important to quantify the effect of promoters.
This study investigates the kinetics of flue gas hydrate in unconsolidated sediments with different particle sizes and quantifies the kinetics of formation, dissociation, and self-preservation using the rocking cell apparatus. Hydrate promoter selected in this study includes three amino acids L-valine, L-methionine, L-histidine amino acids are seen as a potential replacement for toxic surfactants such as sodium dodecyl sulfate (SDS) for gas capture and storage including CH4 and CO2 capture & storage application due to their environment-friendly nature.
Results demonstrate that the presence of hydrophobic amino acids (L valine, L methionine) enhances flue gas hydrate formation and self-preservation effect in different unconsolidated sediments, while hydrophilic amino acids (L-histidine) act as an inhibitor. The difference in behavior is attributed to water perturbation caused by the charge present on the side chain. Smaller particle size enhanced the gas uptake while large particle size lowers the induction time. The presence of porous medium introduces the stochastic nature opposite to bulk water case in the presence of hydrate promoters. Obtained results are expected to provide an enhanced understanding of industrial-scale flue gas capture/storage via hydrate formation in geological formation in the presence of hydrate promoter.

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Fabrication of "sandwich-like"microfluidic chips by ceramic 3D printing for flow visualization experiments

Author: Shidong Li [1]

Co-authors: Sibani Lisa Biswal [2]; Ole Torsæter [3]; Hon Chung Lau [4]; Ludger Paul Stubbs [1]

[1] *Institute of Chemical and Engineering Sciences, Agency for Science, Technology and Research (A*STAR), Singapore*

[2] *Department of Chemical & Biomolecular Engineering, Rice University, United States*

[3] *PoreLab, Norwegian Center of Excellence, Norway. Department of Geoscience and Petroleum, Norwegian University of Science and Technology (NTNU), Norway*

[4] *Department of Civil and Environmental Engineering, National University of Singapore, Singapore*

Corresponding Authors: li_shidong@ices.a-star.edu.sg, ceelhc@nus.edu.sg, ludger_paul@ices.a-star.edu.sg, ole.torsater@ntnu.no, biswal@rice.edu

Microfluidic observation is an important technique for enhanced oil recovery (EOR) studies. It gives insight into two-phase flow in porous media and is also a quick screening tool for different EOR formulations. However, current glass microfluidic chips are costly and complicated to fabricate. This paper explores using 3D printing technology to fabricate the next generation EOR microfluidic chips. First, a stereolithography (SLA) 3D printer was used to test resolution and feasibility of SLA 3D printing for microfluidic chip fabrication. Second, we combined the concept of "sandwich-like"microfluidic chip with ceramic 3D printing to fabricate a "glass-ceramic-glass"microfluidic chip where a ceramic porous medium printed with SLA 3D printer was interlaid between two glass plates. Bonding and lapping technology was applied to bond two glass plates on top and below the ceramic porous medium. The materials used for ceramic 3D printing included alumina, zirconia and fused silica.

In flow visualization experiments using this microfluidic chip, the visibility, maximum pressure, and suitability for EOR experiment were tested, and its wettability was determined by measuring the contact angles between oil, water and the ceramic materials. The surface topography and structure of the ceramic porous medium were characterized by atomic force microscopy (AFM) and scanning electron microscope (SEM). The internal structure of the porous medium was determined by scanning with X-ray micro-tomography.

The SLA 3D printed microfluidic provides a fast, safe and cost-effective way to fabricate a microfluidic chip in the laboratory. The microfluidic chip printed with an SLA 3D printer has a high resolution and acceptable visibility. In addition, it can withstand a relatively high pressure. The "glass-ceramic-glass"microfluidic printed with 3D ceramic printing is a new method to produce microfluidic chip for EOR experiments. The original wettability of the 3D printed ceramic porous medium is water-wet, but can be changed to mixed-wet or oil-wet after aging. The "glass-ceramic-glass"microfluidic chip exhibited good visibility and can withstand high pressure showing promising potential for EOR experiments. In addition, the "glass-ceramic-glass"microfluidic chip has more options for mineral composition potentially (carbonate, clay and mixture of quartz and clay), and is simpler, safer and cheaper to fabricate than a traditional glass microfluidic chip.

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A fractal analysis of stress sensitivity of a porous medium based on the thick-walled Cylinder Model

Authors: Xin Su[1]; Zhaoqin Huang[1]; Jun Yao[1]

[1] *Center of multiphase flow in porous media, China university of Petroleum (East China)*

Corresponding Authors: yaojunhdpu@126.com, suxin_upc@163.com, huangzhqin@upc.edu.cn

How to describe the stress sensitivity of reservoirs has always received much attention. Since the fractal theory was introduced into the reservoirs description, many fractal models have been proposed to evaluate the changes of the porosity and permeability in reservoir with effective stress. In this work, a new conceptual fractal model which combine thick-walled cylindrical model to the solid clusters model porous media is presented. Then based on this conceptual model and fractal theory, a theoretical model of porous media permeability of the porous media is established, which consider the stress sensitivity. The model showed that the permeability of stress-sensitivity porous media is related to the minimum and maximum capillary diameters, Young's modulus and Poisson's ratio of the solid skeleton. Each parameter has a clear physical meaning. Compared with the actual experimental data, it shows better accuracy than the other model, and verifies the validity and correctness of this model.
Keywords：Thick-walled cylinder; Fluid-structure Interaction；FractalPorous Media；Stress Sensitivity；Permeability

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Upscaling of capillary force in simultaneous infiltration of two immiscible fluids through porous media: pore scale LBM modelling

Authors: Zi Li[1]; Sergio Galindo-Torres[1]; Ling Li[1]

[1] *School of Engineering, Westlake University*

Corresponding Authors: s.torres@westlake.edu.cn, liling@westlake.edu.cn, lizi@westlake.edu.cn

The immiscible two-phase flow with both fluids simultaneously infiltrating into porous media plays a crucial role in the processes of oil recovery and non-aqueous-phase liquid mitigation. Therefore, in this study, the dynamics of simultaneous infiltration of immiscible two-phase flow at the steady state in the capillary force-dominated regime was investigated. Based on the two-dimensional pore-scale simulations using the Shan-Chen multiphase lattice Boltzmann model (LBM), the steady-state interfacial area and capillary pressure versus saturation relationships subjected to saturation history and magnitude of hydraulic gradient were examined. Also, the intrinsic differences in the interfacial area and capillary pressure versus saturation curves between at dynamic equilibrium in the simultaneous infiltration and at quasi-static equilibrium in the fluid displacement were explored.

The hysteresis behaviours of interfacial area-saturation and capillary pressure-saturation curves were captured in the fluid displacement, but absent in the simultaneous infiltration because of the steady-state flow dynamics. The unique interfacial area-capillary pressure-saturation surface at dynamic equilibrium did not tend to overlap with the one at quasi-static equilibrium. The hysteretic capillary pressure behaviour for these two flow patterns was of great theoretical and practical significances. In terms of multiphase physics, the present study supplemented Hassanizadeh and Gray's theory (1993a, 1993b) of unique interfacial area-capillary pressure-saturation surface with a new variable: the flow pattern. On the other hand, it was evident that it is essential in engineering practice to apply the capillary pressure curve obtained under a certain flow condition (simultaneous infiltration or fluid displacement) to the same flow pattern of investigation.

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Mesoscopic modelling of fluid-solid interaction and its effect on permeability estimation

Authors: Zi Li[1]; Sergio Galindo-Torres[1]; Ling Li[1]

[1] *School of Engineering, Westlake University*

Corresponding Authors: s.torres@westlake.edu.cn, liling@westlake.edu.cn, lizi@westlake.edu.cn

The liquid slip flow with a Knudsen number Kn = 0.001–0.1 due to intermolecular interactions at fluid-solid (F-S) interfaces is of great importance to the transport of shale oil and clay water. In the framework of the mesoscopic single-phase lattice Boltzmann method (LBM) combined with a midgrid bounce-back boundary condition, we propose two continuous and exponentially decaying F-S interaction force functions: i) between fluid particles and two confined flat walls (Model-I), and ii) between fluid particles and solid particles for porous media (Model-II) to be responsible for the apparent liquid slip. When the F-S interaction force is repulsive (attractive), the phenomena of positive (negative) slip lengths and fluid slip (damping) can be successfully recovered.

For Model-I, we derive the analytical solutions for density profile, velocity profile, slip length, and permeability ratio, which are directly related to the mesoscale interaction parameters and the size of the gap of the flow channel. Through nondimensionalization of the analytical solutions, we obtain the dimensionless numbers that indicate the key feature of the slip flow system. Reasonable ranges for the F-S interaction parameters are suggested based on the observed range of density ratio (film fluid to bulk fluid). Within the given range, simple relationships between permeability ratios and dimensionless numbers are provided by fitting.

For Model-II, the slip length is found to be independent of shear rate (its constituents including body force, and kinematic viscosity), but dependent on pore geometry (smaller in porous media than in parallel-plate microchannels). Both slip length and permeability ratio follow a power law relationship with interaction parameters (strength and decay length) in porous media.

The two proposed models are both validated by the velocity profiles on hydrophobic surfaces in a benchmark microchannel flow. The permeability ratios estimated analytically with the slip length considered agree well with those calculated from analytical solution (Model-I) or LBM simulation (Model-II). The analytical permeability ratio (Model-I) and the estimated permeability ratio (Model-II) both indicate that they increase (decreases) nonlinearly as the pore diameter decreases, suggesting the great importance of the F-S interaction for narrow parallel-plate microchannels and tight porous media.

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An analysis model for hydraulic fracturing liquid imbibition into shale matrix：coupling molecular interactions and dynamic contact angle

Authors: Han Wang[None]; Yuliang Su[1]; Wendong Wang[2]

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

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

Corresponding Authors: wwdong@upc.edu.cn, wanghan.petro@gmail.com, suyuliang@upc.edu.cn

Spontaneous imbibition and forced imbibition of hydraulic fracturing liquids into the water-wet inorganic matrix and the oil-wet organic matrix are a ubiquitous phenomenon, which has an important influence on tight/shale oil recovery and the groundwater contamination.
In this work, the spontaneous/forced imbibition models in inorganic/organic nanopores are established by considering the pore sizes, the liquid–solid molecular interactions, the dynamic contact angle and the pore size distribution based on the no-slip Hagen–Poiseuille and Young–Laplace equations. The liquid–solid molecular interactions reflect the wettability of pore walls, and that can result in the slip boundary and varying near-wall liquid viscosity. The dynamic contact angle is characterized by molecular-kinetic theories. Then, the imbibition models are validated by comparing with the theoretical analysis and dissipative particle dynamics.
The results show that the spontaneous/forced imbibition length increases with the increase of pore radius and length because of the small hydrodynamic resistance. In inorganic pores, the spontaneous imbibition length decreases with increasing water contact angle on the wall due to decreasing capillary pressure. In organic pores, the forced imbibition length increases with increasing oil contact angle on account of increasing slip velocity and decreasing near-wall oil viscosity.
This theoretical analysis can provide microscopic basics into water imbibing into nanopores, and provide guiding information for the oil recovery from tight/shale reservoirs by hydraulic fracturing, the groundwater remediation by restricting imbibition rate and other relevant applications.

KEYWORDS: hydraulic fracturing liquids; spontaneous imbibition; forced imbibition; molecular interactions; dynamic contact angle; slip boundary

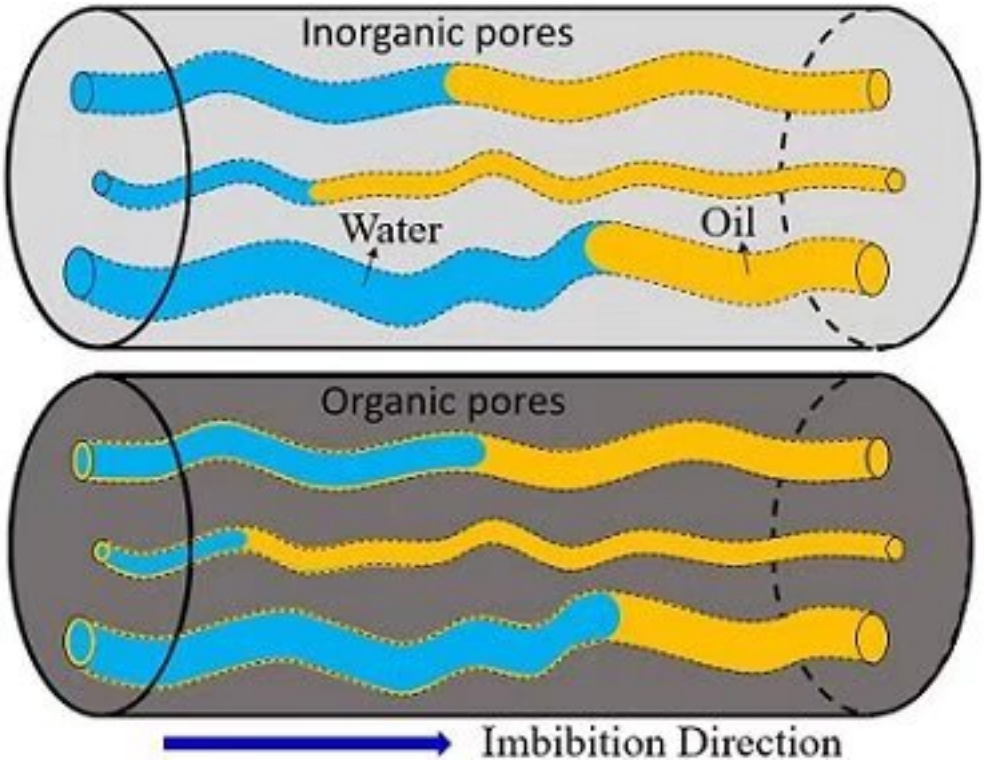

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Fig. Schematic diagram of imbibition process in capillary bundle model

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Multiphase flow in deformable media

Authors: Dawang Zhang[1]; Bjornar Sandnes[1]

[1] *SWANSEA UNIVERSITY*

Corresponding Authors: 936575@swansea.ac.uk, b.sandnes@swansea.ac.uk

Multiphase flows exist extensively in nature and are important in numerous geological and geotechnical applications, such as magma flow, methane leakage from underground and ocean floor, soil remediation, and natural gas and oil extraction. We study experimentally the displacement of one fluid by another(either higher viscous fluid or lower viscous fluid) in deformable solid media contained in the Hele-Shaw cell. Invasion patterns vary in different systems. Invasion of water(higher viscous fluid) into the hydrophobic beads packing saturated in the air(lower viscous fluid) will lead to single fingering and multi-fingering patterns caused by the interface instability. We study the effects of volume fraction of the packing and the effects of the invasion rate of water on the characteristic finger width. We use the principle of the minimization of the work to analyse the experimental results and propose a theoretical model to predict the characteristic finger width and the prediction matches well with the experimental data. Invasion of air into the granular material packing saturated by water will lead to more invasion patterns. At low or quasi-static invasion rate of air, labyrinth or frictional fingering and bubbling patterns happen at the granular packing with low volume fraction or frictional fluids, capillary fracturing happens at medium volume fraction, say 0.58, and capillary fingering happens at relatively rigid packing where friction is larger than pore-enter pressure. At high invasion rate, viscous fingering and capillary fracturing happen at different volume fraction.

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Lattice Boltzmann-pore network hybrid modelling of gas transport in nanoporous media

Authors: Wenhui Song[1]; Maša Prodanović[2]; Christopher J. Landry[2]; Jun Yao[3]

[1] *Research Centre of Multiphase Flow in Porous Media, China University of Petroleum (East China),*

[2] *Hildebrand Department of Petroleum and Geosystems Engineering, The University of Texas at Austin*

[3] *Research Centre of Multiphase Flow in Porous Media, China University of Petroleum (East China)*

Corresponding Authors: song_wen_hui@hotmail.com, rcogfr_upc@126.com, masha@utexas.edu, christopher.landry@utexas.edu

Gas transport in nanoporous media is controlled by both the nanoscale transport mechanisms and complex pore structure. The direct simulation method can accurately capture the detailed gas transport behaviour. However, it is not feasible to apply direct simulation method to the large size sample because of the high computation cost and long computation time. To deal with this, a local-effective-viscosity multi-relaxation-time lattice Boltzmann-pore network coupling model (LEV-LBM-PNM) is proposed in this work to efficiently predict gas transport in complex nanoporous media. The pore network model was extracted from Focused Ion Beam Scanning Electron Microscopy (FIB-SEM) image using the max sphere method. We ran a large number of LEV-LBM simulations in very well resolved geometries with simple cross-sections that had surface roughness added to them in a controlled manner. Such carefully selected geometries were run at a large number of pressure conditions in order to establish gas flux formulas that depend on shape, Knudsen number and surface rougness and can be directly used in PNM in order to account for all of those properties. The benefit of this is that, even in cases where detailed geometry is available for LEV-LBM simulation, our previous study shows that it needs to be magnified up to 5 times (Landry et al 2016) which makes accurate simulation too costly. The semi-analytical gas transport models for single pore with various cross sections and surface roughness were established based on the LEV-LBM simulation results. The established semi-analytical gas transport model is then implemented into the three dimensional pore network model to investigate the gas transport behaviour at various conditions. We found that the proposed LEV-LBM-PNM can accurately predict gas apparent permeability by accounting for gas slip in irregular pore shape and surface roughness.

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Estimating Flow Characteristics of 3D Fracture Network based on Persistent Homology

Authors: Anna Suzuki[1]; Miyuki Miyazawa[1]; Takatoshi Ito[1]; Peter Kang[2]

[1] *Tohoku University*

[2] *University of Minnesota*

Corresponding Authors: anna.suzuki@tohoku.ac.jp, takatoshi.ito.c5@tohoku.ac.jp, miyuki.miyazawa.s8@dc.tohoku.ac.jp, pkkang@umn.edu

Fracture structure of rock dominates the flow of water. Because of the complexity of fracture network patterns, efforts to quantify fracture geometries have been ongoing for decades. Many of them focused on the geometry, which was insufficient to describe the relationship with fluid flow because information of connectivity or tortuosity is necessary for flow properties. Topological data analysis is a rapidly growing field of research, and it provides a set of topological and geometric tools

to infer relevant features from complex data. Persistent homology is one method for computing the topological features of shapes and functions, which provides complex and multiscale geometric information in large datasets. Given that such detailed geometric information would be difficult to be found by simple pattern-matching approaches, persistent homology has been applied in several research fields. This study applies persistent homology to fracture network patterns in order to understand the relationship between flow properties and fracture structures. Several 3D fracture network patterns were generated to conduct direct flow simulation. The fracture network patterns were analyzed by persistent homology. We found the relationship between the persistent homology parameters and fracture structures by a data-driven approach.

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Assessment of Conglomerate Reservoir for CO2 Sequestration using X-ray CT image Analysis

Author: Gidon Han[1]

Co-authors: Weon Shik Han [1]; Kue-young Kim Kim [2]; Jize Piao [3]

[1] *Department of Earth System Sciences, Yonsei University*

[2] *Korea Institute of Geoscience and Mineral Resources*

[3] *Yonsei University*

Corresponding Authors: hang@yonsei.ac.kr, kykim@kigam.re.kr, hanw@yonsei.ac.kr, piaojz@yonsei.ac.kr

Naturally and anthropogenically released CO2 will need to be reduced for mitigating climate change. To mitigate environmental impacts from increased atmospheric CO2 concentrations, geologic carbon sequestration (GCS) is considered as a solution. In GCS, one of the most important things is to identify the properties of reservoir rock material. Previous studies related to GCS have focused on evaluating sandstone reservoirs due to their relatively high porosity and permeability. This study evaluated the petrophysical properties of conglomerate using X-ray CT image analysis.
Characteristics of pore and fluid flow were evaluated using CT image analysis and numerical simulation module for two of conglomerate cores (Core I and II). As comparing two cores, the conglomerates were characterized to be highly heterogeneous; dependent on clast positions and sizes, the number and volume of pores were different even in core samples collected from the same wellbore. The analysis of X-ray CT images revealed the total number of pores (Core I: 59,255 and Core II: 216,787) and pore volume (Core I: 7,409.54 mm^3 Core II: 17,525.83 mm^3). Based on the reconstructed pore space, intrinsic permeability of Core I and II were evaluated implementing fluid simulation (1.18E-12 m^2 to 1.01E-10 m^2); here sub-volumes of pore space were categorized to be 3 groups; (1) matrix, (2) combination of matrix and clast, and (3) fracture within clast. Also, vertical (z-axis) and horizontal (x-axis) permeability were calculated, which showed anisotropic characteristics dependent on the heterogeneity of conglomerate. Finally, the multi-phase fluids simulation for CO2 and groundwater was conducted to evaluate the effect of heterogeneity of conglomerate on migration and distribution of CO2.

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Multiscale flow simulation of shale oil considering hydro-thermal process

Authors: Zijie Wang[1]; Jun Yao[2]

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

[2] *Research Centre of Multiphase Flow in Porous Media, School of Petroleum Engineering, China University of Petroleum (East China)*

Corresponding Authors: rcogfr_upc@126.com, zijie_upc@163.com

The nanopores in shale matrix is complicated, consisting of oleophilic intragranular pore in organic matter and hydrophilic intergranular pore as well as micro fractures in inorganic matter. More than 60% of shale oil will be adsorbed on the surface of organic nanopores with pore size less than 5nm and adsorption behavior of shale oil has significant impact on ultimate oil recovery based on the results of molecular simulation. However, the key point of shale oil production is still focus on free oil, and the boundary slip and multi-layer adsorption have not been thoroughly explored. In this paper, a fully coupled hydro-thermal model is established to investigate the effect of thermal process on enhancing oil recovery (EOR) for shale reservoir, in which the impact of temperature on slip length and the density of adsorbed oil are considered. The results under different stimulation temperatures verify that the thermal enhanced oil recovery through hydraulic fracture heating is an economically feasible method. The adsorption oil production is more sensitive to temperature than free oil. The sensitivity analysis is also conducted on the influence of formation factors and fractal parameters on cumulative shale oil production.

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Pore-scale imaging with measurement of relative permeability and capillary pressure on the same reservoir sandstone under water-wet and mixed-wet conditions

Authors: Ying Gao[1]; Ali Q. Raeini[1]; Ahmed Selem[1]; Igor Bondino[2]; Martin J. Blunt[1]; Branko Bijeljic[1]

[1] *Imperial College London*

[2] *TOTAL E&P France*

Corresponding Authors: y.gao15@imperial.ac.uk, a.qaseminejad-raeini09@imperial.ac.uk, a.selem18@imperial.ac.uk, igor.bondino@total.com, m.blunt@imperial.ac.uk, b.bijeljic@imperial.ac.uk

Using micro-CT imaging and precise differential pressure measurements, we simultaneously measured relative permeability and capillary pressure on a reservoir sandstone sample under water-wet and mixed-wet conditions during steady-state waterflooding experiments. This novel method allows us to elucidate the two-phase flow mechanisms and changes in pore occupancy by comparing our results for two wettability states of the same rock sample.
First, oil and brine were injected through the water-wet reservoir sandstone at a fixed total flow rate but in a sequence of increasing brine fractional flows. Micro-CT images were taken for each fractional flow, while the differential pressure was measured. In the next stage, the surface wettability of the sandstone was altered after prolonged contact with crude oil. Finally, we repeated the same micro-CT imaging and differential pressure measurement procedures on the altered-wettability sample as previously conducted in the water-wet sandstone experiment. Using the pore-scale images acquired under water-wet and mixed-wet conditions, the interfacial curvature was calculated from which the local capillary pressure was obtained. Furthermore, the relative permeabilities were determined from the imposed fractional flow, the image-measured saturation, and the differential pressures. Lastly, the interfacial area and contact angle were calculated to compare the two-phase fluid configurations under water-wet and mixed-wet conditions.
A generalized pore network of the sample was extracted to characterize the pore space geometry and local fluid occupancy of individual pores and throats. We then use this analysis to demonstrate how differences in wettability and occupancy on a pore-by-pore basis affect relative permeability and capillary pressure.
The pore-scale fluid distributions, relative permeability and capillary pressure measured for two wettability states on the same rock sample, will be used to benchmark and validate pore-scale models. This imaging and analysis methodology can be applied to study various other porous medium problems, including fuel cells, water and vapour transport in plants, and carbon dioxide storage.

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Evaporative Salinization in Porous Media

Author: Emna Mejri[1]

Co-authors: Rainer Helmig [2]; Rachida Bouhlila [1]

[1] *National Engineering School of Tunis*

[2] *University of Stuttgart*

Corresponding Authors: rachida.bouhlila@enit.utm.tn, ojalamjr@hotmail.com, rainer.helmig@iws.uni-stuttgart.de

Keywords: Porous Media, Evaporative salinization, Numerical Modeling
Abstract
Evaporative salinization from porous media is a major problem in relation with various environmental and civil engineering issues. The most important environmental concerns are groundwater scarcity and soil quality degradation. These are enhanced by current climatic change (mainly by the increase of temperature inducing the increase of evaporation rates) and the intensive irrigation practices in arid and semi-arid regions.
The main objective of this work is to develop a numerical simulation tool which is used to describe the flow and reactive transport processes related to the evaporation induced soil and groundwater salinization under natural hydro-climatic conditions 2.
Thanks to the developed porous-medium model, we analyze the spatial and temporal evolution of evaporation and multiple salt precipitation processes related to a Tunisian oasis field. The fundamental laws of multi-component mass transport and basic multiple salts precipitation reaction kinetics

are used to construct the model which is implemented in the numerical modeling framework and open source simulator DuMux 1.
This model is currently being extended and coupled with a free-flow sub-model to take into account the influence of climatic conditions on the processes at the free flow-porous medium interface [3]. The coupled model, validated against experimental results, serves as a predictive tool for two environmental issues. The first one being the prediction of soil and groundwater salinization enhanced by salt recycling processes in irrigated Tunisian oasis. The second issue is related to the impact of evaporation-driven salinization on the damage of monuments in an archeological site in Tunisia.

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MULTISCALE PORE NETWORK INTEGRATION USING THE PORE-FLOW SOFTWARE

Author: Elizabeth May Pontedeiro[1]

Co-authors: William Godoy [1]; Marianna Dantas [1]; Fernanda Hoerlle [1]; Martinus Th. van Genuchten [2]; Amir Raoof [2]; Paulo Couto [3]

[1] *LRAP/UFRJ*

[2] *UU/NL*

[3] *LRAP/UFRJ*

Corresponding Authors: bettymay@petroleo.ufrj.br, marianna.silva@coc.ufrj.br, fernandahoerlle@petroleo.ufrj.br, rvangenuchten@hotmail.com, a.raoof@uu.nl, wmgodoy@petroleo.ufrj.br, pcouto@petroleo.ufrj.br

The complex pore structure of carbonate reservoir rocks may be studied by extracting a pore network from 3D X-ray microtomography (microCT) images. The network as defined by its topology and geometry then comprises pore bodies linked by connections (pore throats). The pore network extracted from a rock image must be realistic enough to allow multiphase flow modelling of the system. Combining microCT imaging with pore network modelling (PNM) involves a compromise between sample size and resolution of the scans. Since the pores of carbonate rocks are complex and may vary from sub-microns to centimeters, the samples are often scanned with different sizes and resolutions. One challenge is how to combine information from the different levels in a comprehensive way to better understand flow in the pore network. In our approach we extracted the network from the same sample using different scales of microCT imaging and combining the results in one overall digital pore network using the PoreFlow software 1. The approach permits one to construct reliable 3D multiple-scale models of the porous medium of complex rocks, while maintaining a full description of the real pore structure.
In this study we describe the architecture of the digital model to reconstruct 3D reservoir rocks from 2D thin section images using distinct image resolutions. The method was used to integrate the multiscale pore structure of a coquina plug that is similar to the PreSalt carbonate reservoir rock in Brazil. The skeleton was extracted from microCT images and the permeability was calculated using PoreFlow. Statistical distributions were for this purpose applied to the microCT throat lengths and the pore and throat radii, while connectivities were assigned to the pore bodies. The methodology

was validated by comparing the original network extracted from the reservoir and the network generated using PoreFlow, both in terms of the structural and petrophysical properties of the coquina. As an example, we used the microCT from the coquina plug 1_34A, scanned with a resolution of 18 microns, and compared the PoreFlow digital network with the skeleton obtained from the microCT images. We modeled both skeletons with the PoreFlow PNM software, with results showing good agreement visually and also regarding the parameter statistics. The relative error was 12.6% for the porosity as evaluated by PoreFlow, 3.6% for the permeability, 1.2% for the number of pore bodies, and 1.4% for the volume of the rock. We compared also the mean pore radius (7.3% relative error), the mean throat radius (0.3%) and the mean throat length (1.6%). The next step is to perform the same simulations for two other plugs using microCT images at better resolution. By using the lower resolution skeleton as the main skeleton, we will use the other two skeletons to obtain a more complete pore network at the higher resolution.

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Pore-scale study of complex transport phenomena in porous media

Author: Li Chen[1]

Co-authors: Kang Qinjun [2]; Wen-Quan Tao [1]

[1] *Xi'an Jiaotong University*

[2] *Los alamos Naitonal Lab*

Corresponding Authors: wqtao@mail.xjtu.edu.cn, lichennht08@mail.xjtu.edu.cn, qkang@lanl.gov

Multiphase flow and reactive transport processes in porous media are widely encountered in energy and environment sciences. Typical examples include fuel cells, oil/gas exploitation, CO2 sequestration, thermalchemical storage, etc. The reactive transport processes usually take place at the pore scale (inside the pores or at the interfaces between different constituents), the length scale of which is significantly lower than the length scale of the continuum models based on which transport processes in porous media are usually described. To fill the gap between the two distinct scales, a sets of intrinsic relationships or empirical models are heavily employed to close the continuum-scale models for porous media. However, the validation or accuracy of these relationships/models should be greatly improved to enhance the prediction capacity of the continuum-scale models.
For the past 10 years, we devote ourselves to studying at the pore-scale the transport processes in porous media. Advanced pore-scale tools have been developed including reconstruction of realistic porous structures and constituents of porous media, pore-scale numerical models based on the lattice Boltzmann method for multiphase reactive transport in porous media, and upscaling schemes of pore-scale results into continuum-scale models. The transport phenomena of each process at the pore-scale are investigated and the coupled mechanisms between different processes are revealed. Effects of porous structures, size, interface, and constituents on the multiphase flow and reactive transport processes inside the micro/nanosize pores are deeply explored. Based on the pore-scale numerical results and experimental results, it is revealed that some of the intrinsic relationships or empirical models widely adopted in the literature, predict not only quantitatively but also qualitatively wrong results. Based on the pore-scale results, either these relationships /models are improved

or completely new relationships/models are proposed to enhance the predication capacity of current continuum-scale models for the transport processes in porous media.

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Topological analysis of 3D Discrete Fracture Networks: a graph approach to connectivity and percolation in fractured rocks

Authors: TAWFIK RAJEH[1]; Israel CAÑAMON[2]; Rachid ABABOU[3]; MANUEL MARCOUX[1]

[1] *Institut de Mécanique des Fluides de Toulouse (IMFT), CNRS & Université de Toulouse*

[2] *ETSI de Minas y Energía Departamento de Ingeniería Geológica y Minera (Universidad Politécnica de Madrid)*

[3] *Institut de Mécanique des Fluides de Toulouse (IMFT)*

Corresponding Authors: tawfikrajeh@gmail.com, ababou@imft.fr, marcoux@imft.fr, israel.canamon@upm.es

This work presents a framework to analyze geometrical, topological and hydraulic properties of 3D Discrete Fracture Networks (DFN). A set of efficient algorithms has been developed to perform geometrical and topological analyses upon 3D networks of planar fractures with various shapes (mainly circular and ellipsoidal). The present set of algorithms is capable of (i) calculating all possible intersections in the 3D networks, and calculating also the resulting trace lengths, the fracture areas inside a parallelepipedic domain, and other geometrical attributes of the DFN; (ii) extracting the percolating clusters and eliminating dead end clusters; and (iii) constructing the corresponding graph of the 3D network of planar fractures. The resulting DFN graph can then be used to solve the flow.
All the calculations implemented in the algorithms have been strictly validated by direct numerical calculations or simulations, which increase the confidence in our algorithm methodology. The innovations of the present approach concern mainly (a) the adaptation of the multiple labelling techniques for the search of clusters to the case of 3D DFN's of planar fractures, and (b) the use of efficient algorithms to eliminate dead end clusters in 3D DFN's. Furthermore, the numerical efficiency is highlighted.
Several important applications of the toolbox have been explored. Three of these applications are presented. Firstly, the geometrical analysis capabilities of the toolbox enable finding correlations between 2D attributes such as cumulated trace lengths and 3D attributes of the DFN such as the its connectivity. This application is interesting especially on the construction of relatively realistic 3D networks from 2D observations. Secondly, the graph representation of the DFN enables studying the percolation phenomena in 3D. The recent advances concern mainly the effect of local anisotropy and the mixture of the fracture shapes on the critical density of percolation. Thirdly, it was demonstrated that the use of these algorithms as a pre-treatment (extracting the percolation network, eliminating all dead-end fractures and clusters, searching for shortest paths), considerably reduces the CPU time of flow/transport simulations. The gain on CPU time was several orders of magnitude for networks containing thousands of fractures, and 3D networks containing tens of thousands of fractures are handled in moderate computational time.

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A novel approach towards understanding pore attributes of shale

Authors: Debanjan Chandra[1]; Debanjan Chandra[2]

Co-author: Vikram Vishal [1]

[1] *Indian Institute of Technology Bombay*

[2] *IIT Bombay*

Corresponding Authors: debanjanchandra@iitb.ac.in, v.vishal@iitb.ac.in, rsshantu@gmail.com

Micro and mesopores are dominant fractions of the total porosity in unconventional reservoir rocks that significantly govern the potential for CH4 production and CO2 injection. Among popular methods for determining the pore size distribution (PSD) of shales, low-pressure gas adsorption using N2 (for mesopores) and CO2 (for micropores) as probe gas is widely accepted for probing open/accessible pores. Small-angle neutron/X-ray scattering (SANS/SAXS) is another effective method, which can penetrate into both accessible and inaccessible pores. Determining the PSD of natural samples are not free of complexities. The theoretical isotherm kernel for calculating PSD using density functional theory (DFT) is developed using pure adsorbent, whereas the total porosity in shale/coal is contributed by both organic matter (carbon-based) and clay minerals (silica-based). This study uses a combination of both silica-based and carbon-based models on ten shale samples collected from different depths in Raniganj Basin, West Bengal, India. The objectives of this study are: (a) optimizing the DFT method based on adsorbate-adsorbent interaction and pore shapes for calculating micro- and mesopores, (b) comparison between DFT and grand canonical Monte-Carlo (GCMC) PSD model for calculating micropore distribution, (c) combining the N2-DFT PSD of both Si and C based model for correct estimation of mesopore distribution with further inclusion of CO2-DFT PSD of micropores for total pore volume, (d) depth-wise variation of the change in pore attributes.
Key results are: (a) 66% to 100% increase in pore volume in 3-30 nm pore size bin when used N2-Si+C (quenched solid) QSDFT model compared to only N2-C model. (b) Lesser fitting error in the PSD calculation when the N2-QSDFT-adsorption model is used compared to conventional (non-local) NLDFT models. A better fitting is obtained when CO2-GCMC is used for micropore PSD instead of conventionally used CO2-DFT model. (c) Increased degree of multimodal PSD with optimized N2-QSDFT model indicating the inclusion of all pore width bins. (d) Stitching CO2-DFT and N2-QSDFT model for PSD from 0.3-40 nm pore width. (e) The relation between pore volume, organic matter and abundance of clay minerals was established w.r.t depth. (f) PSD obtained from modified model validated with PSD obtained from small-angle neutron scattering measurements of the same samples at ambient condition. Observation indicates percentage of inaccessible pores decreases with increasing pore size, indicating reduced pore connectivity at the smaller pore size range.

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Numerical Analysis of Interaction between a Reacting Fluid and a Moving Bed with Spatially and Temporally Fluctuating Porosity

Authors: Alban ROUSSET[1]; Abdoul Wahid MAINASSARA CHEKARAOU[1]; Xavier BESSERON[1]; Bernhard PETERS[1]; Chiara GALLETTI[2]

Co-author: Maria Grazia GALLO [3]

[1] *University of Luxembourg, FSTC*
[2] *University of Pisa, DICI*
[3] *Enel Green Power*

Corresponding Authors: chiara.galletti@unipi.it, wahid.mainassara@uni.lu, alban.rousset@uni.lu, xavier.besseron@uni.lu, bernhard.peters@uni.lu

The purpose of this study is to propose a numerical approach that combines low computational costs through the use of high computing efficiency, allowing the realistic use of the design with a sufficient result's accuracy for industrial applications to investigate biomass combustion in a large-scale reciprocating grate.

In the present contribution, a Biomass combustion chamber of a 16 MW geothermal steam superheater, which is part of the Enel Green Power "Cornia 2" power plant,is being investigated with high-performance computing methods. For this purpose, the extended discrete element method (XDEM) developed at the University of Luxembourg is used in an HPC environment, which includes both the moving wooden bed and the combustion chamber above it. The XDEM simulation platform is based on a hybrid four-way coupling between the Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD). In this approach, particles are treated as discrete elements that are coupled by heat, mass, and momentum transfer to the surrounding gas as a continuous phase. For individual wood particles, besides the equations of motion, the differential conservation equations for mass, heat, and momentum are solved, which describe the thermodynamic state during thermal conversion. The grate system has three different moving sections to ensure good mixing of the biomass parts and appropriate residence time. The primary air enters from below the grate and is split into four different zones. Furthermore, a secondary air is injected at high velocity straight over the fuel bed through nozzles. A Flue Gas Recirculation is present and partly injected through two jets along the vertical channel and partly from below the grate.

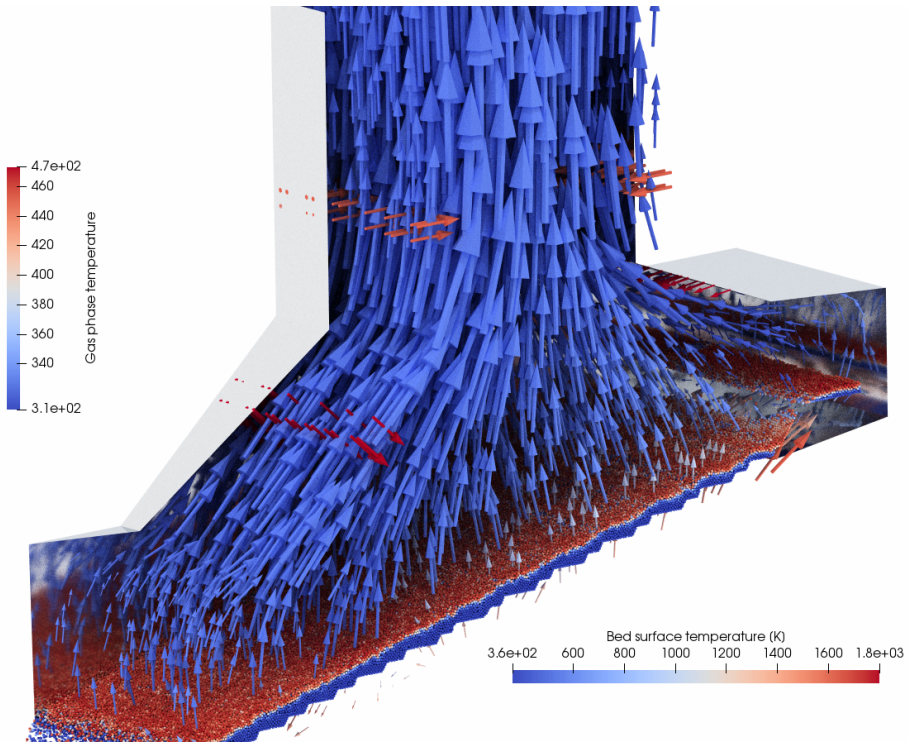

Figure 4: Velocity arrow, bed surface and gaseous phase temperature

The numerical 3D model presented is based on a multi-phase approach. The biomass particles are taken into consideration via the XDEM Method, while the gaseous phase is described by CFD with

OpenFOAM. Thus, the combustion of the particles on the moving beds in the furnace is processed by XDEM through conduction, radiation and conversion along with the interaction with the surrounding gas phase accounted for by CFD. The coupling of CFD-XDEM as an Euler-Lagrange model is used. The fluid phase is a continuous phase handled with an Eulerian approach and each particle is tracked with a Lagrangian approach. Energy, mass and momentum conservation is applied for every single particle and the interaction of particles with each other in the bed and with the surrounding gas phase are taken into account. An individual particle can have a solid, liquid, gas or inert material phases (immobile species) at the same time. The different phases can undergo a series of conversion through various reactions that can be homogeneous, heterogeneous or intrinsic (drying, pyrolysis, gasification and oxidation).

Our first results are consistent with actual data obtained from the sampling of the residual solid in the industrial plant. Our model is also able to predict gas flux behaviour inside the furnace, particularly the flue gas recirculation on the combustion process injection.

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Physically-based combined model for water retention of cementitious materials

Authors: Walaa Issa[1]; Jean-Philippe Carlier[2]; Nicolas Burlion[2]

[1] *Université De Lille LaMCube*

[2] *Université de Lille LaMCube*

Corresponding Author: jean-philippe.carlier@polytech-lille.fr

In all approaches of sustainability of cementitious materials, water plays a key role. Its presence causes the hydration of cementitious binders and greatly influences the properties of concrete as a porous media. In addition to dimensional changes induced by desiccation withdrawals 1 and changes

in the mechanical behavior [2, 3], water saturation of the network also influences the transport properties of cementitious materials.
It is thus of great importance to be able to model and predict sorption isotherms of such materials, which link the water saturation degree of a porous material (Sw) to the relative humidity of the environment (RH) and thus to capillary pressure pc.
The existing models used to represent such relations in the literature (see [4] for a review), generally require the estimation on seldom physically-based parameters through fitting. The objective of this study is to propose a new theoretical model of the sorption isotherms which parameters are related to characteristics of the material (type, formulation and microstructural, hydric and thermodynamic characteristics) that can be easily measured or estimated.
Using such a physically based model would allow the prediction of the retention properties of cementitious materials at different temperatures without performing long water vapour sorption experiments, either by gravimetric sorption or dynamic balance method [5].
The proposed model relies on the distinct consideration of the two main states of water in the porous network, where water can be either adsorbed or capillary condensed.
Capillarity is assumed to occur in the largest pores (capillary porosity). This capillary porosity consists of two porous modes, the large and small capillary pores. Capillary condensation during desaturation is modelled using the bimodal Kosugi model proposed by Seki [6] :
S_w=1/2 [w_1 erfc(ln(p_c/p_(c_MD1))/(√2 σ_1))+w_2 erfc(ln(p_c/p_(c_MD2))/(√2 σ_2))]
With p_(c_(〖MD〗 *i*)) *being the capillary pressure corresponding to the median pore radius of ith fraction of the material, and* ⊠*i a dimensionless parameter to characterize the width of the ith part of pore-size distribution. These parameters are deduced from mercury intrusion porosity curves considering a lognormal distribution of each pore mode.*
Adsorption occurs at the surface of porous materials. We consider then that this phenomenon occurs is the micropores and in an (adsorption) layer on the walls of the capillary pores. This adsorption porosity is determined from the water porosity measurement and from mercury intrusion porosity also considering a lognormal distribution of the pores.
The desorption process of the adsorbed layer is modelled by the three-parameter BSB model [7]:
S_w=(CKW(m*) RH)/(1-K*RH)(1+(C-1)K*RH)

The parameter Wm, related to specific surface of the material, is deduced from the pore size distribution curve.
The parameters C (related to energy released during adsorption) and k (related to energy required for multilayer adsorption) represent the effect of thermodynamics; they are fixed for each type of material based on experimental data, considering an exponential evolution as a function of temperature.
The new combined model proposed here allows the prediction of the isothermal desorption curves of cementitious materials at moderate temperatures without the need for parameter calibration.

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Lattice Boltzmann Simulations for micro-macro interactions during isothermal drying of porous media

Authors: Debashis Panda[None]; Supriya B[None]; Vikranth Kumar Surasani[1]

[1] *BIrla Institute of Technology and Science*

Corresponding Author: surasani@hyderabad.bits-pilani.ac.in

It is a demanding task to elucidate the influence of pore-scale dynamics to the up-scaled features in multiphase applications of porous medium. One such complicated multiphase application is considered in this work i.e. the drying of porous medium. As drying is analogous to two-phase imbibition process in a porous medium 1, phenomena like Haines jumps 2, Capillary Valve effect (CVE) [3], film-effects [4] and sudden invasion of pores (bursting and merging invasion) [5] influences the up-scaled drying kinetics of the porous medium. Moreover, the pore-structure is also an essential factor in differentiating the various periods of up-scaled drying kinetics i.e. constant rate period and falling rate period. In past, pore-scale approaches, namely PNM [6] has been used to understand such micro-macro interactions in the drying of porous media but it failed to elucidate the influence of Haines jumps, influence of cohesive and adhesive forces for film formations etc. Thus, in this work, we present a novel approach to understand the micro-macro interactions for drying of porous media i.e. Lattice Boltzmann Methods (LBM) [7]. LBM is a mesoscale approach which plays as an interface by solving the Navier-Stokes equation at macroscale and imitate the pseudopotential intermolecular forces at microscale. The establishment of micro-macro interactions of drying of porous medium is as follows: First, a one-dimensional representation of the porous medium is considered i.e. bundle of capillaries, to elucidate the influence of pore distribution (i.e. mono-modal and bi-modal) and the dominance of capillary and viscous forces to the up-scaled drying period i.e. constant rate period and falling rate period. Next, we consider a two-dimensional porous medium to present the influence of pore-scale activities like Haines jumps, CVE and film effects to drying of porous medium. These pore-scale activities are observed in a chronological order. First, the CVE is observed, which leads to a delay in the invasion of the pore. Next, due to contact angle instability and CVE, bursting and merging invasion is observed. Finally, the Haines jumps is observed which leads to sudden fluctuation in the drying kinetics and the fluctuation decays as the saturation of water decreases with prolonged period of time. These observations captured using LBM and the attempt to track the up-scaled drying rates renders LBM as a powerful multiphase CFD tool for intricate application of drying of porous medium.

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Stochastic and upscaled analytical modeling of fines migration in porous media induced by low-salinity water injection

Author: Yulong Yang[1]

Co-authors: Weifeng Yuan [1]; Jirui Hou [1]; Zhenjiang You [2]; Jun Li [1]

[1] *China University of Petroleum, Beijing*

[2] *The University of Queensland*

Corresponding Authors: lijun446@vip.163.com, yuanweifeng_0121@163.com, zhenjiang.you@gmail.com, yulong.yang@cup.edu.cn, houjirui@126.com

Fines migration induced by injection of low-salinity water (LSW) into porous media can lead to severe pore plugging and consequent permeability reduction. The deep-bed filtration (DBF) theory is used to model the aforementioned phenomenon, which allows us to predict the effluent concentration history and the distribution profile of entrapped particles. However, the previous models fail to consider the movement of the waterflood front. In this study, we derive a stochastic model for fines migration during LSW flooding, in which the Rankine–Hugoniot condition is applied to calculate the concentration of detached particles behind and ahead of the moving water front. A downscaling procedure is developed to determine the evolution of pore-size distribution from the exact solution of a large-scale equation system. To validate the proposed model, the obtained exact solutions are used to treat the laboratory data of LSW flooding in artificial soil-packed columns. The tuning results show that the proposed model yields a considerably higher value of the coefficient of determination, compared with the previous models, indicating that the new model can successfully capture the effect of the moving water front on fines migration and precisely match the effluent history of detached particles.

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A comparative study of Lattice Boltzmann models for complex fractal geometry

Author: Dong Zhang[None]

Co-authors: Xiaoli Liu ; Enzhi Wang

Corresponding Author: zhangd18@mails.tsinghua.edu.cn

Abstract:
Lattice Boltzmann Method(LBM) is currently utilized for mesoscopic fluid simulation with second-order accuracy in space and time. Compared with other Computational Fluid Dynamics(CFD) methods, LBM is preferred for simplicity of implementation and predestination to massively parallel computing 1, especially in complex geometries, such as Newman and Timothy utilized LBM to investigate the single-phase flow inside 2D and 3D porous media [2, 3]. However, Navier-Stokes(N-S) equation is derived from lattice Boltzmann equation(LBE) via Chapman-Enskog expansion with the relative error O(Ma2)and Ma is Mach number, especially for incompressible limitations[4].To improve the accuracy and efficiency, different models (standard D2Q9, He-Luo model and D2G9 model[5]), collision operators(single-relaxation-time(SRT), two-relaxation-time(TRT) and multiple-relaxation-time(MRT)[6]), boundary conditions (BCs, such as standard bounce-back, half-bounce-back and immersed boundary[7]) are proposed, and comparative study were conducted. However, the objective of study mentioned are 2D Poiseuille flow, lid-driven square cavity flow and couutte flow, all geometries are simple, besides majority of researches investigating flow inside porous media with complex geometry utilized the original and simplest LBM model, thus accuracy of results is doubtful. In this paper, porous media with complex geometry is constructed by Sierpinski carpet, different MRT-LBM model with same BCs and finite element method(FEM) are utilized for simulate single-phase flow inside porous media, then a systematically and quantitatively comparative study is conducted to evaluate the accuracy of different methods and investigate the effect of grid and pressure drop on the results, which will provide guidance and suggestions for simulation of real porous media.

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Microfluidic Observations and Pore-Scale Simulations of Fluid Displacement and Capillary Trapping Under Intermediate-Wet Conditions

Author: Rumbidzai. A. E Nhunduru[1]

Co-authors: Amir Jahanbakhsh [1]; Omid Shahrokhi [1]; Krystian. L Wlodarczyk [2]; Duncan. P Hand [2]; William. N MacPherson [2]; Susana Garcia [1]; M. Mercedes Maroto-Valer [1]

[1] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, UK*

[2] *Applied Optics and Photonics Research, School of Engineering and Physical Sciences, Heriot-Watt University, UK*

Corresponding Authors: m.maroto-valer@hw.ac.uk, a.jahanbakhsh@hw.ac.uk, d.p.hand@hw.ac.uk, w.n.macpherson@hw.ac.uk, k.l.wlodarczyk@hw.ac.uk, o.shahrokhi@hw.ac.uk, s.garcia@hw.ac.uk, ran4@hw.ac.uk

Capillary trapping (also known as residual trapping) which leads to the immobilization and isolation of fluid ganglia in porous media is common to many subsurface engineering applications, including carbon dioxide (CO2) sequestration. Capillary trapping is highly desirable and of great importance in CO2 sequestration applications as the trapping of super-critical CO2 in the interstitial spaces of porous rocks inhibits plume migration and enhances storage safety and capacity(1)(2). Capillary trapping can contribute up to 40% of the overall CO2 trapping in the first 100 years post injection (3) and is strongly influenced by the wettability of the porous medium (1)(4).

Capillary trapping of CO2 has been studied extensively in water-wet systems, mostly sandstone reservoirs, however this trapping mechanism has not been thoroughly investigated for intermediate and oil-wet reservoirs in which pore-scale capillary forces related to the fluid displacement process would undoubtedly be different from that of water-wet systems (5).

Likewise, in this study the intrinsically water-wetting surfaces of micromodels, manufactured from glass plates (6), were chemically altered to mimic intermediate-wet reservoir conditions through the use of surface modification agents. Imbibition experiments were conducted using two analogue CO2-brine fluid pairs; deionized (DI) water and n-decane as well as DI water and air. The fluid displacement mechanisms associated with the imbibition processes were investigated and residual fluid saturations for different porous structures were quantified. Pore-scale simulations were also conducted using the Volume of Fluid method in OpenFOAM (7). Results from the micromodel experiments were used to validate the simulation results. Fluid displacement at intermediate wettability was compared with water-wet conditions.

This work shows that fluid displacement during the imbibition process under intermediate-wet conditions occurs through a series of cooperative pore-filling events. The type (isolated, throat, cross linked or dead end) and size of pores present in the porous structure was found to have a great influence on residual trapping under intermediate-wet conditions. The presence of dead-end pores promoted residual trapping of the non-wetting fluid. The combination of these experimental and simulation studies provides a unique insight to multiphase flow at intermediate wet conditions.

Acknowledgements
This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (MILEPOST, Grant agreement no.: 695070). This paper reflects only the authors'view and ERC is not responsible for any use that may be made of the information it contains.

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An investigation of caprock-cement integrity for CO2 storage

Author: Amir Jahanbakhsh[1]

Co-authors: Jonaid Hasan Bajwa [2]; Nazia Mubeen Farooqui [2]; M. Mercedes Maroto-Valer [3]; Mojgan Hadi Mosleh [4]; Harshit Agrawal [5]; Anna Korre [5]; Sevket Durucan [5]

[1] *Research Centre for Carbon Solutions, School of Engineering and Physical Sciences, Heriot-Watt University*

[2] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University*

[3] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, UK*

[4] *Lecturer at the University of Manchester*

[5] *Department of Earth Science and Engineering, Royal School of Mines, Imperial College London*

Corresponding Authors: h.agrawal17@imperial.ac.uk, mojgan.hadimosleh@manchester.ac.uk, a.jahanbakhsh@hw.ac.uk, s.durucan@imperial.ac.uk, a.korre@imperial.ac.uk, m.maroto-valer@hw.ac.uk, jhb1@hw.ac.uk

The long-term integrity of wellbores has been a technical risk for CO2 geological storage 1. Cement degradation due to exposure to CO2-saturated formation water is of great concern with respect to wellbore integrity. The reactions between CO2-saturated formation water with minerals in the cement and rock result in mineral dissolution and/or mineral precipitation which can directly affect wellbore integrity 2. Therefore, it is critical to thoroughly understand the interactions between rock/cement and fluids in a CO2 storage system. In this work, we used composite cement-caprock core samples and performed a series of experiments simulating deep wellbore conditions to study the effect of CO2-saturated brine on chemical, physical and mechanical properties of the samples [3,4]. The composites were exposed to CO2-saturated brine for three periods of 3, 6 or 9 months using hydrothermal vessels at pressure and temperature of 250 bars and 90^oC, respectively. To carefully analyse the samples, we performed X-ray Micro-Computer Tomography (µCT) and petrophysical evaluation (porosity, permeability) and geo-mechanical testing (mechanical and elastic properties).

Using X-ray µCT, 3D volumes of the composite samples were reconstructed, and Figure 1 shows the reconstructed volume of an individual void space before and after CO2 exposure 5. 2D images from the reconstructed models obtained before and after exposure of the composite sample to CO2-brine solution (250 bars and 90^oC) were analyzed qualitatively to ascertain the extent of the physical and chemical changes. It was clearly observed that small cracks were filled by mineral precipitation. Pore-scale analysis showed that both precipitation and dissolution mechanisms have been active during the exposure time. As a result of precipitation, a clear reduction in the volume of the void space in individual pores was observed. Petrophysical and geo-mechanical analysis showed a significant reduction in permeability of the composite samples after the long-term exposure to CO2-brine solution; however, the effective porosity and mechanical properties of the cement and caprock, as well as the bond between them, were not affected significantly.
The integration of X-ray µCT and permeability measurements showed that dissolution and precipitation of some minerals started from early stage of exposure. The high-permeable small cracks in the cement were filled as the result of precipitation and/or carbonation and reduced the composite permeability significantly. This phenomenon may help mitigate against leakage at reservoir pressure and temperatures considered in this research.

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Acknowledgements
This research was carried out as part of the UK Research Councils'Energy Programme funded consortium project "CO2 Injection and Storage-Short and Long-term Behaviour at Different Spatial Scales"

, Grant Reference: EP/K035967/1. The authors would like to thank financial support from the Robert M Buchan Chair in Sustainable Energy Engineering at Heriot-Watt University. The authors would also like to thank Dr. Sean Higgins at RCCS for taking the micro CT images.

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Quasi-3D pore-scale simulation of wettability heterogeneity in porous media

Author: Amir Jahanbakhsh[1]

Co-authors: Omid Shahrokhi [2]; M. Mercedes Maroto-Valer [3]

[1] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences Heriot-Watt University*

[2] *Heriot-Watt University*

[3] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, UK*

Corresponding Authors: m.maroto-valer@hw.ac.uk, o.shahrokhi@hw.ac.uk, a.jahanbakhsh@hw.ac.uk

Wettability plays a crucial role in multiphase flow and fluid displacement in porous media [1,2] and it is generally classified as homogeneous and heterogeneous [3]. For homogeneous wettability, the whole rock surface has a uniform molecular affinity for the fluids in contact. In contrast, for heterogeneous wettability, variation in affinities for the fluids at different regions is expected [3]. Most reservoirs display heterogeneous wettability which can be categorized as either fractional or mixed-wet [4]. In the fractional-wet group, oil- and water-wet regions are random with respect to pore size, but in mixed-wet group water- and oil-wet pores are sorted based on their size 5.
In order to understand the effect of wettability heterogeneity at the macroscopic level on flow functions, e.g. relative permeability and capillary pressure, it is essential to understand its role at microscale/pore level. Limited micromodel studies have been performed on microscale wettability heterogeneity mainly due to fabrication challenges [1,6]. Significant impacts on fluid displacement and level of residual saturation have been observed in the system with non-uniform wettability 1. Although fabrication of porous media replicas with several spatial configurations for wettability heterogeneities is not practical, pore-scale numerical simulations are very useful to study different scenarios and optimize the experimental design for further investigation.
To the best of our knowledge, most of the numerical simulation studies investigated the effect of different uniform wettability on fluid flow dynamics, however, most of the rocks display heterogeneous wettability (fractional or mixed-wet). In this work, we have used direct numerical simulations (DNS) to investigate wettability heterogeneity at pore-scale. DNS studies were conducted using the Phase Field method using a commercial computational fluid dynamics (CFD) software (COMSOL Multiphysics) [7]. We have built Quasi-3D pore-scale models and simulated homogenous and heterogeneous types of wettability and investigated the effect of uniform and non-uniform wettability

on the two-phase flow in porous media.
Two-phase flow displacements are compared at different uniform and non-uniform contact angles distributions. We observed that non-uniform wettability has a significant effect on the evolution of fluid interface, pressure drop across the system, displacement efficiency and trapped saturation. A porous media with equal surface areas of two different contact angles e.g., 60° and 120° does not simply behave similar to a media with a uniform contact angle of 90°. Simulation results showed that certain spatial configurations of wettability heterogeneity at microscale assist the stability of displacement, while other configurations promote flow instability for the same pore-scale geometry. The results of these DNS studies are of interest to different subsurface processes involving wettability alteration and reactive transport.

Acknowledgement
This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (MILEPOST, Grant agreement no.: 695070). This paper reflects only the authors'view and ERC is not responsible for any use that may be made of the information it contains.

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Probabilistic Modeling of Halite Nucleation and Growth in Porous Media: Pore Scale Modeling

Authors: Mohammad Masoudi[1]; hossein fazeli[2]; Rohaldin Miri[3]; Helge Hellevang[4]

[1] *University of Oslo, Department of Geosciences*

[2] *University of Oslo*

[3] *Iran university of science and technology*

[4] *Department of Geosciences, University of Oslo*

Corresponding Authors: helge.hellevang@geo.uio.no, rohaldinmiri@iust.ac.ir, mohammad.masoudi@geo.uio.no, hossein.fazeli@nottingham.ac.uk

Mineral nucleation and growth during reactive transport in porous media, results in the changes in the porosity and permeability. The place of the nucleation of the secondary minerals and the way that the formed nucleus grow in porous media have major effects on the porosity-permeability relation. On the other words, in order to have a precise prediction of the hydrodynamic of the porous media after precipitation of secondary mineral, first we need to predict where in the pore space the secondary minerals nucleate and how they grow. Mineral nucleation is a probabilistic process,

where crystals can nucleate anywhere given the same physical conditions (surface characteristics, supersaturation, temperature, etc). Therefore, a probabilistic approach is required to understand how permeability and fluid flow may change following mineral dissolution-growth.
In this work, we develop a new probabilistic nucleation model and incorporate it into a pore-scale reactive transport solver to simulate the mineral nucleation and growth in the porous media. The model is used to simulate halite nucleation and growth in a capillary tube that is initially filled with NaCl brine. The concentration of NaCl in the top boundary increases with time and halite mineral can nucleate anywhere in the tube. The model is run several times to get different patterns for porosity-permeability relation. The more frequent porosity-permeability relation is suggested to be used for modeling of well injectivity during carbon storage process.

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Microscopic flow behavior of foam in porous media and its effect on oil displacement efficiency

Authors: yj ji[1]; ll w[1]

[1] *Southwest petroleum university*

Corresponding Author: jiyoujun0319@163.com

Abstract: According to the numerical experiments, microphenomenon produced by foam migration in complex pore throat was studied. Firstly, the single-capillary model is used to analyze the Jamin effect caused by deformation and stretching, Snap-off mechanism and coalescence mechanism when the foam passes through the narrow pore throat. Meanwhile, the micro-selective migration mechanism of foam moving in complex pore throat was analyzed. Secondly, by mans of CT image processing technology, microscopic pictures of porous media are identified, the pore structure is divided into solid regions and fluid regions, and real microscopic numerical models of porous media are erected, moreover, foam migration process in porous media is simulated. In the end, the profile and plugging performance of different types of foams in porous media were evaluated.
The results indicate that the pressure of the foam when passing through the pore throat is related to the degree of foam deformation, the surface tension is proportional to pressure, meanwhile, the inverse of pore throat radius is linear correlation with the pressure, foam has priority in large pore at a micro level, the foam system in the porous media showed strong stability. The flow characteristics of foam in porous media are mainly manifested in plugging pores with low resistance to make the streamline more uniform. These results will provide useful enlightenment for the profile control and flooding by using gas-liquid dispersion on site. Based on this study and the actual geological characteristics of XB oilfield, a kind of foam with better profile and plugging performance was selected.

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Radionuclide transport and retention at the core scale identified by GeoPET analysis and reactive transport modeling

Authors: Tao Yuan[1]; Johannes Kulenkampff[1]; Till Bollermann[1]; Cornelius Fischer[1]

[1] *HZDR, FS Leipzig*

Corresponding Authors: t.yuan@hzdr.de, c.fischer@hzdr.de, t.bollermann@hzdr.de, j.kulenkampff@hzdr.de

Low-permeability Opalinus clay formations are considered as a potential host rock for the storage of high-level nuclear waste (Nagra 2002). The diffusion of dissolved species is the dominating transport process in this rock type (Van Loon et al. 2003). Stratification and spatial variability of composition cause anisotropic and heterogeneous diffusion patterns, which could significantly speed up diffusive transport compared to commonly assumed homogeneous conditions. Anisotropy of diffusive transport has been studied on oriented samples in diffusion cells and with positron emission tomography (Kulenkampff et al. 2016). The heterogeneity of the diffusive spreading is increased still further due to sandy layers and diagenetic carbonates, affecting the radionuclide migration behavior at the core scale.
Here, we parameterize a reactive transport model by using experimental and analytical data on Eu(III) sorption efficiency at the pore scale. The effective retention coefficients calculated at the pore scale serve as input values for the reactive transport simulation at the core scale. Diffusive transport model parametrization utilizes GeoPET/µCT results on the migration behavior of 22Na+ at the core scale. Numerical simulation is performed using an existing code (Yuan et al. 2019), which contains the reactive transport model for simulating reactive diffusion process at the core scale. The combination of pore-scale reactivity and core scale transport modeling provides critical insight into the radionuclide migration heterogeneity. We discuss these results with a focus on upscaling strategies to the field scale of host rocks.

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Giant Piezoelectrolytic Actuation in Nanoporous Silicon-Polypyrrole Membranes

Authors: Manuel Brinker[1]; Guido Dittrich[1]; Thelen Marc[1]; Lakner Pirmin[2]; Claudia Richert[3]; Tobias Krekeler[1]; Thomas F Keller[2]; Norbert Huber[3]; Patrick Huber[1]

[1] *Hamburg University of Technology*

[2] *Deutsches Elektronen-Synchrotron (DESY)*

[3] *Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht*

Corresponding Authors: patrick.huber@tuhh.de, manuel.brinker@tuhh.de

The absence of piezoelectricity in silicon makes electro-mechanical applications of this mainstream semiconductor impossible. External electrical control of the silicon mechanics, however, would open up entirely new perspectives for on-chip actuorics. Here, we employ wafer-scale, self-organized

nanoporosity in silicon in combination with polymerization of an artificial muscle material (polypyrrole) inside pore space to synthesize a material that shows macroscopic electrostrain. As we explore by macroscopic dilatometry and synchrotron-based x-ray diffraction experiments on the crystalline lattice of the silicon pore walls the material expands and contracts reversibly under electrical potential control when immersed in an aqueous electrolyte. The voltage-strain coupling parameter is 3 orders of magnitude larger than the best-performing piezo ceramics. By a micromechanical analysis we trace this huge electroactuation to the concerted action of 100 billions of parallel nanopores per square centimeter cross-section and to potential-dependent pressures of up to 150 atmospheres at the single-pore scale. The exceptionally small operation voltages (0.3-0.8 V) along with the biocompatibility and the facile synthesis of the material pave the way for silicon-based (bio-)actuorics.

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Ionic liquid dynamics in nanoporous carbon: A pore-size- and temperature-dependent neutron spectroscopy study on supercapacitor materials

Authors: Mark Busch[1]; Tommy Hofmann[2]; Bernhard Frick[3]; Jan Embs[4]; Boris Dyatkin[5]; Patrick Huber[1]

[1] *Hamburg University of Technology, Ei{\ss}endorfer Stra{\ss}e 42, 21073 Hamburg, Germany*

[2] *Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany*

[3] *Institut Laue-Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France*

[4] *Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, 5232 Villigen, Switzerland*

[5] *Department of Materials Science and Engineering, A. J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, PA, 19104, U.S.A.*

Corresponding Author: patrick.huber@tuhh.de

The influence of spatial confinement on the thermally excited stochastic cation dynamics of the room-temperature ionic liquid 1-N-butylpyridinium bis-((trifluoromethyl)sulfonyl)imide ([BuPy][Tf_2N]) inside porous carbide-derived carbons with various pore sizes in the sub- to a few nanometer range are investigated by quasi-elastic neutron spectroscopy. Using the potential of fixed window scans, i.e. scanning a sample parameter, while observing solely one specific energy transfer value, an overview of the dynamic landscape within a wide temperature range is obtained. It is shown that already these data provide a quite comprehensive understanding of the confinement-induced alteration of the molecular mobility in comparison to the bulk. A complementary, more detailed analysis of full energy transfer spectra at selected temperatures reveal two translational diffusive processes on different time scales. Both are considerably slower than in the bulk liquid and show a decrease of the respective self-diffusion coefficients with decreasing nanopore size. In spite of this dynamic slowing down we can show that the temperature range of the liquid state upon nanoconfinement is remarkably extended to much lower temperatures, which is beneficial for potential technical applications of such systems.

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Surface probing with Streaming Potential: The Polymer Flooding Scenario

Authors: Michael LEVANT[1]; Nicolas AGENET[1]; Enric SANTANACH-CARRERAS[1]

[1] *TOTAL S.A.*

Corresponding Authors: enric.santanach-carreras@total.com, michael.levant@total.com, nicolas.agenet@total.com

In this work we present the first experimental evidence of polymer adsorption in natural limestones, obtained by direct surface probing via measurement of the streaming potential coupling coefficient. We use a recently developed method to demonstrate sign inversion of the brine/rock interface following polymer flooding, - an unambiguous evidence of polymer adsorption that may also imply changes in wettability. This method, to our knowledge, has not been used in polymer flooding scenario. Instead, indirect methods were used to assess the problem of polymer adsorption.
The method consists of a sensitive setup with exceptional signal-to-noise ratio, capable of detecting voltage fluctuations below 0.1 mV even at high salinity (≈3 mol/L model formation brine). We conducted a series of experiments where we measure the coupling coefficient before and after the polymer injection. The injection of partially hydrolyzed polyacrylamide (HPAM) Flopaam 3130S was followed by chase flooding with formation water for several pore volumes, to assure that the «before» and «after» measurements are carried out in the same conditions, and therefore any changes registered after the polymer flooding can be attributed to the adsorbed polymer.
The most significant result is the detection of the adsorbed polymers via the sign inversion of the surface charge following polymer flooding, which can be seen already in the raw experimental data. Therefore this result is an unambiguous evidence for adsorption, beyond merely numerical variations and is also model independent, that was consistently observed in other experiments with polymers of different molecular weight.
This is in accord with the fact that the experimental conditions are particularly favorable for adsorption, i.e. negatively charged HPAM on positively charged surface of limestone in calcium-rich model formation water, and other observations, such as residual resistance factor, and reduced permeability following low salinity flooding due to the swelling of the adsorbed layer.
Finally, our results are not merely an introduction of a new measurement method. Although the sign inversion by itself is not surprising, it has interesting implications on various oil recovery scenario that include injection of additives given that surface charge impacts the wettability.

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Surface Probing with Streaming Potential: The Polymer Flooding Scenario
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https://doi.org/10.1007/s11242-019-01318-7

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Multi-scale Extended Finite Element Method For Fractured Geological Formations

Authors: Fanxiang Xu[None]; Hadi Hajibeygi[None]; Bert Sluys[None]

Corresponding Authors: l.j.sluys@tudelft.nl, h.hajibeygi@tudelft.nl, f.xu-4@tudelft.nl

In the underground resource engineering it is common that the highly valuable resource locates inside the highly fractured geological formations. Underground reservoir fluid pressure change, resulting from either resource extraction or fluid injection, leads to stress field change within these formations. The stress-field change can cause unfavorable surface displacements (i.e., subsidence or uplift) and activate faults and fractures (i.e., induced seismicity). These consequences can lead to growing opposition in the society towards the use of underground resources for supply of affordable energy (e.g., as in hydrocarbon) and renewable energy (e.g. geothermal production and energy

storage). The geological formations span large length scales and are typically highly heterogeneous and massively fractured at different scales. As such, accurate and efficient simulation of mechanical deformation in heterogeneous fractured geological formations is a key factor in maintaining the safety of operations.
For mechanics analysis extended finite element method (XFEM) provides an advantage of avoiding complex meshes. For geoscientific applications, there exists several fractures over large (km) length scales. For such application, having a scalable and accurate XFEM method is extremely important. To achieve this, we present the first multiscale extended finite element (MS-XFEM) method. MS-XFEM develops local multiscale basis functions which allow for constructing accurate coarse-scale systems. These basis functions are computed locally using XFEM. Both enrichment functions along the fracture nodes and tips are considered in the basis function calculation. These functions are then used to construct and solve the coarse-scale system. Note that no enrichment exists on the coarse level. This makes our MS-XFEM procedure computationally efficient, yet accurate, for highly-fractured real-field applications. For several test cases, the MS-XFEM performance is investigated compared with the classical XFEM method. MS-XFEM casts a promising approach for real-field analyses of mechanical deformation influenced by the reservoir pore-pressure change.

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Density Functional Theory Model for Adsorption-Induced Deformation of Materials with Convex Pore Walls

Authors: Andrei Kolesnikov[1]; Gennady Gor[2]

[1] *Institut fur Nichtklassische Chemie e.V.*

[2] *New Jersey Institute of Technology*

Corresponding Authors: gor@njit.edu, andrei.kolesnikov@uni-leipzig.de

Adsorption of fluids in nanoporous media causes mechanical stresses and results in deformation 1. This phenomenon is ubiquitous, and its magnitude depends on the pore size and geometry. Adsorption and adsorption-induced deformation is typically modeled in pores with concave pore walls (cylindrical or spherical pores) or planar geometry (slit pores). However, many porous materials are composed of spherical grains, so that the pores are formed by the intergranular spaces between the convex surfaces. Here we present a first theoretical study of adsorption-induced deformation of materials with convex pore walls. We take the templated mesoporous carbons (CMK-3) which have an ordered hexagonal structure of parallel cylindrical rods 2, and model adsorption of nitrogen in this system using the classical density functional theory (DFT) within the local density approximation. Adsorbed fluid density profile in CMK-3 geometry can be reduced to two dimensions, but unlike slit or cylindrical pore model it cannot be made one dimensional. The fluid-fluid interaction parameters are fit to experimental nitrogen binodal, and reproduce other thermodynamic properties (such as surface tension and vapor pressure). The solid-fluid interaction parameters are fit to reproduce the nitrogen adsorption at 77 K on a reference carbon surface. Using the resulting parameters we predict the adsorption isotherms and strain isotherms for nitrogen adsorption in CMK-3 carbons. The shape of adsorption isotherm matches the shape of experimental isotherm. The predicted strain isotherms are qualitatively different from the strain isotherms in cylindrical pores [3]. We attribute this difference to formation of liquid bridges between the adjacent rods. Our results suggest that adsorption-induced deformation in materials with convex pore walls cannot be predicted within the existing models. These results may shed some light on understanding adsorption-induced deformation of consolidated granular media, such as sandstone [4].

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Sorption characteristics of biomass-based carbonaceous materials for containment of volatile organic compounds (VOC)

Author: Hamid Rajabi[1]

Co-authors: Mojgan Hadi Mosleh [2]; Amanda Lea-Langton [1]; Parthasarathi Mandal [1]

[1] *The University of Manchester*

[2] *Lecturer at the University of Manchester*

Corresponding Authors: partha.mandal@manchester.ac.uk, amanda.lea-langton@manchester.ac.uk, hamid.rajabi@manchester.ac.uk, mojgan.hadimosleh@manchester.ac.uk

Volatile organic compounds (VOCs) emitted from crude oil contribute to air pollution and tropospheric ozone as well as imposing profound adverse effects on human health and well-being. Most of containment strategies developed in recent years require advanced technologies (e.g. thermal and chemical treatments [1, 2]), and therefore are relatively expensive especially for large areas where numerous oil spills have led to vast contaminated lands. Biomass-based adsorbents such biochar are potential sustainable solutions for containment of VOCs due to abandonment of raw materials (e.g. locally available bio-waste from agricultural industry) and relatively low-cost production [3].
In this research, a bespoke experimental facility with an advanced GC-FID analyser has been develop to quantify and study the sorption capacity of various types of biochar to a range of VOCs. Isothermal and kinetic behaviour of gas sorption on biochar is investigated to better understand the mechanisms involved in those processes. The effects of feedstock type and pyrolytic temperature on VOC sorption capacity are investigated and the influential parameters such as pore structure and surface functional groups are discussed in details.

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Application of Laplace Equation to Derive Hydraulic Conductivity from Velocity Measurements in Porous Media

Author: Michael Mont-Eton[1]

Co-author: David Mays [1]

[1] *University of Colorado Denver*

Corresponding Authors: michael.mont-eton@ucdenver.edu, david.mays@ucdenver.edu

Numerical techniques are routinely employed to predict velocity fields in porous media as a function of known or simulated heterogeneous hydraulic conductivity (conductivity) fields. Here we present a method for the inverse problem, to find the heterogeneous conductivity field as a function of known or simulated velocity fields. As an inverse solution, conductivity is possible to obtain using stochastic techniques (Lu and Zhang, 2002), (Chang and Yeh, 2010), parametrization (Jiao and Zhang, 2015a), or Adomian decomposition (Panawalage et al., 2018). All of the above techniques have a similarity: hydraulic head data on the boundaries must be supplemented with additional field data of the same type, and the error for the computed data is dependent on the number of additional observations and the reliability of the observations (Jiao and Zhang, 2015b).

The method is dependent on switching between the use of central summation equations that input velocity data and estimate conductivity, and central difference equations which predict hydraulic head. We use the iterative ADI method (Alternating Direction Implicit method), which is ideally suited to solving elliptic equations on square grids (Kreyszig, 2011), with both forward and backward error analysis to minimize the quantitative difference between known extrinsic data and predicted intrinsic characteristics. The method is demonstrated with a simulated steady, two-dimensional velocity field calculated from assumed isotropic heterogeneous conductivity. The calculated conductivity field reproduces the assumed conductivity field exactly. More generally, by framing this approach as a method to derive intrinsic properties from extrinsic observations, other applications range from fluid mechanics to thermodynamics, gravity and electromagnetics.

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Predicting the effective thermal conductivities of sands using machine learning and a thermal conductance network model

Authors: Wenbin Fei[1]; Guillermo Narsilio[1]

[1] *The University of Melbourne*

Corresponding Authors: narsilio@unimelb.edu.au, wenbin.fei@unimelb.edu.au

Sands are complex granular materials composed of particles varying in size, shape, connectivity and mineral compositions. These microstructural features and the variety of boundary conditions make it challenging to accurately predicting the effective thermal conductivities (ETC) of granular materials. While empirical equations can be established by conducting numerous experiments or numerical simulations, singling out the impact of individual factors on ETC is difficult. Machine learning techniques have been attempted to predict the ETC. However, the materials data are much smaller than other fields, allowing the existing attempts to act as proof of concept for sphere packings and artificial irregular particle packings. Moreover, the existing research has not taken the particle connectivity variables as inputs when training the machine learning model for real sands, which may lead to the difference between the ETC from measurements and models. A sand can be idealised as a network of nodes (particles) and edges (interparticle contacts or/and small gaps between neighbouring particles), from which network features can be extracted. The network features have the merit of capturing both particle connectivity and contact quality (contact area or thermal conductance) which is essential to heat transfer. The networks are also extended to build a thermal conductance network model (TCNM) to calculate the ETC. An artificial neural network (ANN) model is trained to predict the ETC of sands , showing good efficiency and accuracy.

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The Influence of Fractures on the Enrichment of Tight Sandstone Gas

Author: Ping Wang[1]

Co-authors: Quanyou Song [1]; Baogang Li [1]; Wenqing Tang ; Jin Wang [2]

[1] *China University Of Petroleum*

[2] *China University of Petroleum*

Corresponding Authors: 846396194@qq.com, 478684961@qq.com, 1404195190@qq.com

The fracture characteristics of tight sandstone gas reservoir are the dominant factors that affect the difference of reservoir hydrocarbon content. Fractures in tight sandstone gas reservoir can be divided into structural fractures and non-structural fractures according to their genesis. Structural fractures are the main fracture types of low-permeability tight sandstone reservoir in sedimentary basin, which play the most important role in the exploration and development of tight sandstone gas reservoir. Fracture plays a significant role in improving the reservoir space and pore throat structure of tight reservoir. The isolated pores are linked by fractures to form connective reservoir spaces, forms a complex pore-fracture network system, improves the percolation capacity of reservoir, and forms an advantageous channel for gas migration. The fracture can also be used as a place for gas storage and seepage because of its width when it connects the isolated pores. Fractures improve the efficiency of oil and gas filling. The existence of micro fractures provides an advantage channel for gas filling in tight sandstone reservoir, improves the efficiency of gas injection in tight reservoir, and fractures can also increase gas effective permeability , which is conducive to gas seepage. The time and space position of fracture development are different, and the accumulation of tight sandstone gas reservoir is also different.
Key words: fractures ; tight sandstone gas ; gas migration and accumulation

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Pore-scale study of spontaneous imbibition in digital rock by using a color-gradient lattice Boltzmann model

Author: Yang Liu[1]

Co-authors: Jianchao Cai [1]; Qingbang Meng [1]; Xuan Qin [1]; Shanshan Jiang [1]

[1] *China University of Geosciences, Wuhan*

Corresponding Authors: mengqb@cug.edu.cn, 575167537@qq.com, caijc@cug.edu.cn, liuycug@126.com, qinx@cug.edu.cn

Spontaneous imbibition in porous media plays an important role in enhancing oil recovery, especially in unconventional reservoirs with low or ultra-low permeability. Due to the extremely complex structure of natural porous media, no matter by means of micro-experiments or numerical calculation, the pore-scale mechanisms of spontaneous imbibition and its quantitative impacts on dynamic production have not been well understood. In this work, a color-gradient lattice Boltzmann model is used to simulate the spontaneous imbibition process of binary fluid systems with different properties in several groups of digital rocks and the multi-relaxation time scheme (MRT) algorithm is used to improve the numerical stability and accuracy in the whole calculation process. Additionally, a process-based algorithm is introduced to accurately determine and dynamically characterize the distribution of wetting and nonwetting phases in the pore space at different time steps. The flow of binary immiscible fluids in imbibition process with the conditions of different viscosity ratios and contact angles are discussed in depth. Combined with the pore structure distribution characteristics of these digital rocks, such as pore size distribution, connectivity distribution and fractal characteristics, the effects of fluid properties on the distribution of binary immiscible fluids in spontaneous imbibition process and the characteristics of porous media on the final recovery factor are also discussed in depth. The results obtained can provide qualitative and quantitative insights in spontaneous imbibition in naturally fractured resorisers.

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Fractal analysis of shape factor for matrix-fracture transfer function in fractured reservoirs

Author: Lan Mei[1]

Co-authors: Jianchao Cai [1]; Qingbang Meng [1]; Qiuying Sun [1]; Shuang Li [1]

[1] *China University of Geosciences, Wuhan*

Corresponding Authors: meil@cug.edu.cn, sunqy@cug.edu.cn, 13476029236@163.com, caijc@cug.edu.cn, mengqb@cug.edu.cn

A new two phase matrix-fracture transfer function is proposed for fluids flow simulation of fractured reservoirs with dual-porosity models. Most of the existing matrix-fracture transfer function by assuming pseudo-steady state flow, considering part of main mechanisms that control multiphase flow and ignoring the effect of microscopic pore structures on fluids transfer between matrix and fracture. In this study, the complexity of pore structures can be characterized by fractal geometry theory, and a fractal governing equation for pressure diffusion (fluid expansion) and saturation diffusion (imbibition) which can be applied to derive a new form of the transfer function for two phase flow under unsteady state hypothesis is established. The proposed fractal two phase transfer function analytically account for the effect of microscopic pore structures, fluid expansion and imbibition on two phase fluids transfer between matrix and fracture. New shape factors for saturation diffusion are defined. The fractal two phase transfer function is applied to the single block dual-porosity models, which is in good agreement with the numerical simulation results of fine-grid single-porosity models. In this study, many of these existing limitations are removed to help improve understanding of multiphase flow characteristics in fractured systems.

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Fractal analysis of real gas transport in 3D shale matrix

Author: Zhenhua Tian[1]

Co-authors: Jianchao Cai [1]; Yihua Xiong [1]; Haitao Tian [1]; Kai Xu [1]

[1] *China University of Geosciences, Wuhan*

Corresponding Authors: xuk1111@foxmail.com, lingkongdaxia@163.com, tianzh@cug.edu.cn, caijc@cug.edu.cn, tht@cug.edu.cn

Shale gas reservoirs are of low porosity, poor permeability, complex pore structures and complex compositional minerals, and multi-scale effect during the transport of gas which results in the transport characteristics that are different from conventional gas transport theory. The transport mechanisms in the shale gas reservoir have not been well understood by now. Shale gas has a significant role in energy supply in the world due to its substantial deposits. Therefore, it is of great importance for efficient exploitation to clarify the transport mechanisms in the shale matrix.
There are mainly three aspects in the stating of shale gas transport mechanisms by now: experimental study, molecular simulation study, and theoretical model study. The theoretical model study has its advantages because it scarcely can be restricted by experimental apparatus and computing power.
The transport mechanisms of shale gas are different at different pore sizes, temperature and pressure. Based on the Knudsen number (Kn), the flow regimes can be divided into four parts: viscous flow regime, slip flow regime, transition diffusion regime, and molecular diffusion regime. At the in-situ condition, the transport of gas in shale matrix is mainly influenced by viscous flow, slip flow, transition diffusion, and surface diffusion.

In our work, a transport theoretical model for real gas in shale nanopores is built by the linear superposition of bulk transport and surface diffusion firstly. The bulk transport part in our model is consistent with other bulk transport model for comparison. The bulk gas permeability is larger than the Darcy permeability while the pore diameter is less than 10 nm. The bulk gas permeability is close to the Darcy permeability with the increase of pore diameter. The surface diffusion term takes up an important part of the total permeability in small nanopores. Considering the pore size distribution of shale is mainly of nanometer scale, hence the surface diffusion is shale should be considered. Secondly, a coupled fractal transport model in 3D shale matrix is deduced with the help of fractal geometry and fractal capillary tubes model. The fractal transport model is verified by helium permeability and methane permeability. Transition diffusion is important at low pressure while slip flow is dominated at high pressure in shale matrix. The surface diffusion also has contribution to the total permeability to a certain extent.

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A feasible method for the construction of fixed-tortuosity capillary medium with self-similarity behavior

Author: Wei Wei[None]

Co-authors: Jianchao Cai [1]; Yuxuan Xia ; Haitao Tian [1]; Zhenhua Tian [1]

[1] *China University of Geosciences, Wuhan*

Corresponding Authors: tht@cug.edu.cn, tianzh@cug.edu.cn, xiayx@cug.edu.cn, weiwei@cug.edu.cn, caijc@cug.edu.cn

The hypothesis that capillary model represents the real porous system is a proper description of fluid transport characteristics in porous media, while the intrinsic features of tortuous capillary structure are rarely evaluated. In this work, we focus on the issue of the virtualization for tortuous capillary structure. We present a feasible method to construct streamtube of fixed length, and the tube has self-similarity behavior during generating process. The single capillary can be dominated by three parameters, pore fraction (porosity), tortuosity and fractal dimension. For testing the performance of capillary pattern, several cases based on different parameters are used to investigate the feature of tortuous polyline and streamtube. We analyze the relation between tortuosity and fractal dimension, and find the results that there exist at least three types of tortuosity model with the change of fractal dimension. It also emphasizes that the scheme of using multi-capillaries to compose pore connected system is reasonable.

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Elastic equivalent numerical modeling of porous media digital core

Author: Shi-kai Jian[1]

Co-authors: Liyun Fu ; Qiang Liu ; Lijie Cui

[1] *China university of petroleum (East China)*

Corresponding Author: jianshiakai@163.com

Abstract: It is a widespread method to analyze rock elastic properties based on porous media digital cores. Digital core is a three-dimensional high-resolution image of mineral particles and microporous structure of rock samples obtained by using X-ray micro CT technology in a non-destructive method, which can be used to calculate the physical properties of rock (such as elastic modulus, permeability, etc.) and simulate the migration and flow of fluid in the pore and fracture space. Based on the high-resolution Berea sandstone digital core image, the digital core here is divided into quartz matrix and pore space by threshold segmentation method. In this paper, the differential equivalent medium model (DEM), the self-consistent approximate model (SCA), the finite element method (FEM) and the dynamic elastic wave equation are used to perform the equivalent numerical simulation of Berea sandstone. Through the elastic equivalent numerical simulation of Berea porous medium model with the different porosity, the accuracy of calculation results of the above methods can be compared. Then, the appropriate equivalent numerical calculation method can be selected to improve the accuracy of elastic equivalent numerical modeling effectively.
Key words: porous media; digital core; elastic equivalent numerical modeling

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Study on Film effects during isothermal diffusion dominated evaporative drying of square capillary tube using Lattice Boltzmann model

Authors: Supriya B[None]; Debashis Panda[None]; Nicole Vorhauer[1]; Vikranth Kumar Surasani[2]

[1] *Otto-von-Guericke University*

[2] *BIrla Institute of Technology and Science*

Corresponding Authors: surasani@hyderabad.bits-pilani.ac.in, nicole.vorhauer@ovgu.de

Evaporative drying in porous media involves complex inter-linkages between the transport properties in the porous media and the boundary condition that affect the drying kinetics during drying process1. The drying of capillary channels are considered as a fundamental model for construction of pore structures because it enables us to understand the invasion patterns of the air-water interface with evolution of time and the micro-macro interactions in the porous media2. Thus in the present work, the drying phenomena of a liquid confined in a simple geometry of square capillary tube is studied. The real scenario is such that liquid films[3] develop along the tube internal corners under the effect of capillary forces, as the bulk meniscus recedes inside the tube. At the pore-scale, pore-network model revealed the presence of the films using simple geometry[4]. However, PNM has limitations in using true geometry and incorporating the intermolecular forces and in unfolding the film effects. In this work, we present a novel approach of modeling multiphase phenomena i.e. Lattice Boltzmann method (LBM) 5 for the drying of the square capillary tube. LBM is a mesoscale

approach which plays as an interface by solving the Navier-Stokes equation at the macro-scale and the pseudo-potential intermolecular forces at micro-scale. The drying kinetics commonly observed in experimental work of a confined geometry, the constant drying rate period followed by the falling rate period was observed. Then the characteristics of the constant drying rate period and the falling rate period are studied with the effect of the films formed due to the capillarity effects. The liquid transport across the square capillary tube is explained with the pressure gradient which leads to the capillary pumping and the capillarity along the liquid-gas interface at the internal corners of the tube resulting in the formation of the corner films (hydraulic films) and surface films. The hydraulic films are analogous to the micro-throat of the bundle of capillaries which is the main reason for the wetting of the entrance of the tube and contributes to the constant rate period. Whereas, the surface films are the films present on the walls of the tube, which contributes to the formation hydraulic films as the bulk meniscus recedes.

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Insights into Laws of Topology in Wetting

Author: Chenhao Sun[1]

Co-authors: James McClure [2]; Peyman Mostaghimi ; Anna Herring [3]; Steffen Berg [4]; Ryan Armstrong

[1] *University of New South Wales*

[2] *Virginia Tech*

[3] *Australian National University*

[4] *Shell Global Solutions International B.V.*

Corresponding Authors: peyman@unsw.edu.au, ryan.armstrong@unsw.edu.au, chenhao.sun@unsw.edu.au, mcclurej@vt.edu, annalisaherring@gmail.com, steffen.berg@shell.com

Soft matter interfacial phenomena play a central role in numerous natural and technological systems on a daily basis as well as industrial and military applications. We introduce a topological interpretation for the wetting state of fluids and derive general relationships that hold for any soft matter system. We show that topological relationships can be used to derive equilibrium contact angles and demonstrate that the approach succeeds in situations where Young's equation is invalid. We investigate that our developed concept can describe effective wetting behavior in complex and confined domains, which links across various length scales pertinent to wetting phenomena. We link the topological description with thermodynamics and show that it is able to capture effects due to dynamic contact angles, surface roughness and chemical heterogeneity at different length scales. In addition, we show that the developed approach is less sensitive than the direct contact angle measurement at contact points due to gridding and voxelization effects, which can be considered as a robust and consistent method for wettability characterization in complex multiphase systems. Overall, the

approach is applied to interpret complex droplet dynamics that highlight the fundamental role of topology in wetting phenomena, with the perspective of future applications, e.g., design of complex synthetic materials, superhydrophobic surfaces, microfluidics and bio-inspired materials.

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Study on the migration property and the enhanced oil recovery mechanism of nanometer microspheres

Author: Peng Lv[1]

Co-authors: Yigang Liu [1]; Yunbao Zhang [1]; Xianghai Meng [1]; Jian Zou [1]; Leiyang Dai [1]; Huan Xia [1]; Yanyue Li [1]; Nan Wang [1]; Hui Li [1]; Baoqing Xue [1]

[1] *Tianjin Branch of CNOOC (China) Ltd.*

Corresponding Author: hilvp@163.com

As an effective technique for stabilizing oil and controlling water, microspheres flooding has been widely used in Bohai offshore oilfield. Deep migration of microspheres in porous media is a key performance in microspheres'inherent physical and chemical properties which influence the role of microspheres on effecting oil stabilization, blocking up water and tapping the potential oil. The molecular size and structure of a typical nanometer microspheres and the rheological characteristic of the nanometer microspheres solution were briefly studied by particle size instrument, scanning electron microscopy and rheometer in this paper. On this basis, the influence of the nanometer microspheres concentration and hydration time on the migration ability of the nanometer microspheres in sand-packed tube and different injection timing on oil recovery were investigated by displacement equipment with multi-point pressure measuring capability. The displacement mechanism of nanometer microspheres were discussed by bridging theory, colloid and interfacial chemistry theory combined with doublet displacement model 1. The results showed that the initial particle size of the nanometer microspheres was between 300 nm and 600nm at 55℃. The particle size of nanometer microspheres increased continuously with the hydration time when they were hydrated in simulated water. After 20 days hydration, the mean diameter of the normal distribution of nanometer microspheres is 10μm. The nanometer microsphere solution with concentration of 500 ~ 4000mg/L exhibited the characteristics of pseudoplastic fluid at a low shear rate, Newtonian fluid at a medium shear rate and dilatant fluid at a high shear rate. For 1400mD sand-packed tube model, the optimal plugging concentration of the nanometer microspheres was 0.2%. On the conditions the plugging performance of the nanometer microspheres in porous media after different hydration time was studied. When the hydration time was 3 days, the plugging effect was not obvious, while when the hydration time was 7 days, the plugging effect began to show. However, it was quite different from that of the nanometer microspheres after 14 days hydration in which the resistance factor reached 40. As the hydration time increased, the pullging ability of the nanometer microspheres in porous media increased. Slow expansion of nanometer microspheres ensures their injection into the pores of sand-filled tubes.The nanometer microspheres showed well plugging and deep migration ability in pores of sand-packed tube. For 1400mD sand-packed tube model with saturated oil, it improved 8% OOIP by injecting 0.3 Pv nanometer microspheres solution with concentration of 2000 mg/L after the water flooding when the water cut reached 98%. It improved 25% OOIP for the same sand-packed tube model and the same nanometer microspheres slug which was injected in the early displacement stage. Injection timing of nanometer microspheres shows a significant influnence on enhanced oil recovery. Combined with experiment results and doublet displacement model, only expanding and not dissolving in water is the precondition for the nanometer microspheres to play the role of enhancing oil recovery while bridging, adsorption and retention after expansion are the main enhanced oil recovery mechanisms of the nanometer microspheres.This study will promote the further application of microsphere in Bohai.

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The change of reservoir physical properties with formation pressure decreasing and its influence on remaining oil

Authors: Jintao Wu[None]; Yong Hu[None]; Guangming Pan[None]; Jianting Huang[None]; Hao Li[None]

Corresponding Author: wjtwave@163.com

Due to the long-term development with natural energy, severe decrease of the formation pressure has been observed in KQ reservoir. The oil field is a weak volatile oil field locating at Bohai Bay with the underground viscosity of 2.9mPa.S and the original formation pressure of 35.0MPa. After 18 years of development, 8 adjustment wells were drilled while the maximum formation pressure drop reached 15MPa. Compared with the old wells, the physical properties observed in adjustment wells including porosity and permeability became worse and the thickness ratio of the poor reservoir increased obviously. Therefore, two questions are raised: one is whether the change of reservoir physical properties is related to the decrease of formation pressure; the other is how the change of reservoir physical properties affects the remaining oil.

The change of porosity and permeability under different formation pressure is obtained through the laboratory core test. Based on the relationship between pore compression coefficient and effective overburden pressure, a quantitative model of porosity variation with formation pressure is established. The results show that when the formation pressure drops to 10MPa, the formation porosity decreases to 98.1%. For the characterization of permeability changing with pressure, three different models including pressure sensitive method, exponent method and Carmen-Kozeny equation method are used for regression analysis. The results show that Carmen-Kozeny equation method is more applicable and when the formation pressure drops to 10MPa, the permeability decreases to 83.8%.

Based on the above quantitative characterization of reservoir physical properties with the change of formation pressure, the influence of the physical properties change on the remaining oil is studied by numerical simulation. The compaction expansion module in commercial simulator CMG is used to perform the change of porosity and permeability in the actual well group model. The results show that after 18 years of natural energy production, the average porosity decreases to 98.6%, the average permeability decreases to 87.2% and the effective thickness decreases to 94.1%, at which time the formation pressure drops to the lowest level. Moreover, the remaining oil saturation with and without considering the change of physical properties is compared. It can be seen that with considering the permeability change, the remaining oil saturation in the layers with better physical property decreases, while that in the layers with worse physical property increases. The difference of the remaining oil saturation between the layers increases gradually with the development and the maximum difference can reach 3.2%. By discussing the influence of different reservoir parameters, the applicable limits considering the influence of reservoir physical property change are obtained. The inflexion value is selected as the limit value and the limit range is permeability < 300mD, permeability range > 5, formation pressure drop > 5MPa.

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Distribution and Quantitively Evaluation of Micro Residual Oil after Polymer Flooding based on CT Scanning

Author: Liu TAO[None]

Co-authors: Yongfei Yang [1]; Jun Yao [2]; Lei Zhang [3]; Hai Sun [2]

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

[2] *Research Centre of Multiphase Flow in Porous Media, School of Petroleum Engineering, China University of Petroleum (East China)*

[3] *China University of Petroleum*

Corresponding Authors: zhlei84@163.com, s18020157@s.upc.edu.cn, sunhaiupc@sina.com, rcogfr_upc@126.com, yangyongfei@upc.edu.cn

As traditional water flooding being limited to enhance oil recovery, polymer flooding plays an important role in oil industry. In this study, we carried out a series of experiments of water flooding and polymer flooding based on artificial sandstones with the aid of CT scanning. By using image processing techniques, we visualized the displacement process and got quantitively evaluation of the microscopic residual oil distribution and morphological change at different displacement stage. We discussed the differences between water flooding and polymer flooding in enhance oil recovery, and find that polymer can help to change the flow path and the viscoelastic of polymer also help to drive the droplets in the corner and small pores that water hard to sweep out. After polymer flooding, oil phase presents a more dispersed distribution, and more oil was displaced. By setting up different control-experiments, we studied impact of permeability and injection speed on oil recovery of polymer flooding. The results show that enhanced oil recovery after polymer flooding for the cores with the permeability of 3989×10-3μm2, 1543×10-3μm2 and 813.6×10-3μm2 can be 10.13%, 6.30% and 4.34%, respectively. Meanwhile, when it comes to higher injection speed, the oil recovery rate can also be improved. Thus, different enhance oil recovery methods can be applied to the field according to the results and conclusion.

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Microstructure characterization and permeability modeling of creeping porous media under various pressures

Author: Yuxuan Xia[1]

Co-authors: Jianchao Cai [2]; Sai Xu [1]; Haitao Tian [1]; Yang Liu [1]

[1] *China University of Geosciences, Wuhan*

[2] *China University of Geosciences (Wuhan)*

Corresponding Authors: caijc@cug.edu.cn, liuycug@126.com, tht@cug.edu.cn, xus@cug.edu.cn, xiayx@cug.edu.cn

Creeping porous media (e.g. soil, loose sandstone and clayey-silt stone) has the characteristics of non-diagenesis, poor cementation, high clay mineral content, and low median grain size. When developing such reservoirs, the pore space will be compressed under high pressure, resulting in permeability reduce. In this study, the water seepage experiments under different pressure gradients are carried out using the clayey-silt sediments of natural gas hydrate reservoir at the Shenhu Area in the South China Sea, in which the sample was subjected to computed tomographic (CT) scans. The experimental results and CT images show that the creeping porous media has a compression of the pore structure and decreasing permeability with the increasing pressure. The pore structures are characterized by several parameters through fractal geometry theory. It is found that there is an obvious negative linear relationship between pressure and structural parameters including

porosity, average pore and throat radius, pore and throat median radius, maximum pore and throat radius, and fractal dimension. On the basis of fractal capillary assumption, a creeping structural permeability model for natural gas hydrate reservoir is then established by including pressure effect. The presented model provides a theoretical frame for permeability changes under various pressures of creeping porous media.

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SEM, Raman and Micro-CT characterization of CO2–Induced Wellbore Cement degradation

Authors: Yan WANG[None]; Liwei Zhang[1]; Xiuxiu Miao[2]; Manguang Gan[None]

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

[2] *State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences*

Corresponding Authors: ywang@whrsm.ac.cn, cumtgmg@163.com, zlw_85@foxmail.com

Wellbore cement integrity under CO2 geologic storage (CGS) conditions is a key factor to assure safe and permanent storage of CO2. Wellbore cement integrity may be impaired and the structure of cement may be altered as a result of CO2 attack. To understand how CO2-induced structure alteration in oil well cement under CGS conditions affects well integrity in CGS projects, this paper reports an experiment of reaction between CO2 and oil well cement under CGS conditions. Samples were scanned by Micro CT before and after reaction. The Micro CT is capable of operating at 140KV and 10W, has a maximum resolution of 10μm. To simulate the reaction between CO2 rich brine and oil well cement at CGS conditions, our team has developed a testing system which provides the storage temperature and pressure.

The samples were made by standard class G oil well cement used for CGS pilot projects. The cement was cured at CO2 storage formation conditions: 62℃, 17MPa, and 1 wt% NaCl solution. The curing was maintained for 14 days. The diameter of the samples was 10 mm. Every sample contained a small borehole at center (around 1 mm diameter) that made the samples suitable for examining seepage through small leakage pathways within cement. During the reaction experiment, the samples were placed in the high-pressure, high-temperaure testing system for 14 days, given a temperature of 62℃ and a CO2 partial pressure of 17MPa. The goal of this experiment is to evaluate how the geochemical reactions between dissolved CO2 and cement affect structure of the cement. Change of borehole geometry was not observed in the Micro CT images. However, a region with decreased porosity around the borehole due to CaCO3 precipitation and a region with increased porosity around the borehole due to Ca(OH)2 and C-S-H dissolution were observable. Initial distribution of cementitious materials and solution buffering governed the width of the high-porosity region and CaCO3 precipitation region. This study demonstrates a 3-D sample characterization technique that can be used to investigate CO2-induced structure alteration of oil well cement.

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Investigation of the flowing rules and interface condition of coupled two phase porous medium flow and free flow

Authors: Long Huang[1]; Zhaoqin Huang[1]

[1] *Center of multiphase flow in porous medium, China university of Petroleum (East China)*

Corresponding Author: 1428452927@qq.com

Abstact：
The spatial structure of fractured vuggy reservoirs is complex and multi-scale. Establishing accurate mathematical models to describe the flow rules and the two-phase motion interface are difficult points in the study of the mechanism of two-phase flows in fractured vuggy porous media. During the flow of fluid from the porous medium region into the vuggy region, it will form droplets on the wall surface of the porous medium, and detachment and merge from the wall surface. The current macro-scale model has not yet considered this flow process. On the pore scale, the relatively small area of the coupling interface between porous medium and vuggy is analyzed, and the microscopic coupling flow law of coupling tow phase porous medium flow and free flow can be accurately studied by solving the Navier-Stokes equation. On the pore scale, the pore network model is used to model and characterize the porous medium. The two-phase flow interface phenomenon and flow law between the porous media and the vuggy are studied under different geometric structures. Based on the micro-scale study, upscaling to macro scale and establishing the two-phase macroscopic interface condition of coupled two phase porous medium flow and free flow to realize the macroscopic numerical simulation of fractured vuggy reservoirs.

Key words:
porous medium flow and free flow, fractured vuggy porous media, two phase, flowing rules, interface condition, upscaling

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Adsorption and Flow Behaviors of Shale Oil in Organic Slit by Molecular Simulation

Author: JIe Liu[1]

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

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

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

Corresponding Authors: s18020122@s.upc.edu.cn, yangyongfei@upc.edu.cn, shenliu603@163.com

Shale oil is widely distributed in organic nanopores, while kerogen plays a complex and key role for adsorption behavior of shale oil, and thus it is crucial to identify the associated storage and transport mechanisms. In this work, the molecular dynamics simulation had been performed to quantify the adsorption and flow behavior of shale oil in kerogen slits. Both the distribution of shale oil properties and potential of the mean force (PMF) were used to identify the interaction mechanisms between the light and heavy components respectively represented by methane and asphaltene. We also examined the effects of different temperatures and apertures on the adsorption behavior. The rough kerogen channels contribute to the heterogeneous viscosity and unconventional differentiation of velocity. Owning to the extremely strong adsorption capacity between the asphaltene and kerogen, the adsorbed asphaltene layers reduce the slit width, preventing the light components from adsorbing on the kerogen slits due to the energy barrier formed by heavy components. It is found

that the medium components are the most potential fraction in thermal exploitation, and the light components keep a steady quantity with the combined action of medium and heavy components. The micro slit (aperture < 2 nm) can be blocked by asphaltene molecules, and the adsorption density of hydrocarbons reaches the maximum at 2 nm aperture.

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Numerical simulations of biofilms in core samples: MEOR and MICP

Author: David Landa Marbán[1]

Co-authors: Gunhild Bødtker [2]; Bartek Florcsyk Vik [2]; Per Pettersson [2]; Iuliu Sorin Pop [3]; Kundan Kumar [1]; Florin Adrian Radu [4]; Svenn Tveit [2]; Sarah Gasda [5]

[1] *University of Bergen*

[2] *NORCE Norwegian Research Centre*

[3] *Hasselt University*

[4] *University of Bergen, Norway*

[5] *NORCE Energy*

Corresponding Authors: kundan.kumar@uib.no, bavi@norceresearch.no, sorin.pop@uhasselt.be, pepe@norceresearch.no, florin.radu@uib.no, svtv@norceresearch.no, gubo@norceresearch.no, sarah.gasda@norceresearch.no, david.marban@uib.no

A biofilm is an aggregate of microbes enclosed in a matrix of primarily polysaccharides, generally referred to as extracellular polymeric substance (EPS). Biofilms produce acids, biomass, gases, polymers, solvents and biosurfactants. In addition, biofilms can induce the precipitation of calcium carbonate in a calcium-rich environment. Biofilms are complex systems, involving different physical, chemical and biological processes such as bacterial decay, endogenous respiration, erosion, sloughing, abrasion, attachment, bacterial reproduction and formation of metabolites. Biofilms are present in many systems, with beneficial applications in some areas, for example in medicine, food industry, climate change, oil recovery and water quality.

In our research, we are interested in studying biofilms for two different applications: microbial enhanced oil recovery (MEOR) and microbially induced calcite precipitation (MICP). The former consists on using the biomass for the bioplugging technology to improve oil recovery whereas the latter consist on using the biofilm for calcite precipitation to prevent leakage of sequestered CO2. In this work, we develop core-scale models for permeable biofilms including bacterial growth, death, attachment and detachment. The transport of components is governed by convection and dispersion. The biomass reduces the rock porosity and hence the rock permeability.

Core-scale experiments are important as they allow us to conduct studies (i.e., permeability reduction over time, diverse injection techniques, oil recovery for different system setups) at reservoir conditions (i.e., real rock samples, pressure, temperature). Core-scale models are important as they aim to calibrate parameters from experimental data to perform field-scale simulations and study diverse injection techniques to optimize the results.

The developed mathematical model for bioplug technology includes two phases (water and oil), one nutrient, and biofilm formation on the pore walls. We discuss the outcomes of the numerical simulations to experimental results. We present a novel global sensitivity analysis to identify the critical parameters in this mathematical model. Diverse porosity-permeability relationships for evolving pore space can be found in literature. We consider two empirical relationships for permeable biofilm and two derived effective relationships derived by upscaling (Landa-Marbán et al.). Finally, we present

the results of three different studies: impact of porosity-permeability relations on the oil recovery, impact of diverse injection strategies on the oil recovery and the sensitivity analysis.

The developed mathematical model for MICP accounts for single-phase flow (water), transport of three components (urea, bacteria and nutrients) and two mass balance equations (biofilm and calcite). Numerical simulations are presented in a core using parameters reported in literature and we compare the results to experimental data reported by Ebigbo et al. (2012). Diverse injection techniques are studied to compare different permeability reductions in a core-sample with thief zones.

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The Seebeck effect in membrane systems of ions abundant in seawater

Authors: Kim Kristiansen[1]; Peder Holmqvist[1]; Signe Kjelstrup[2]

[1] *PoreLab NTNU*

[2] *PoreLab, Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway*

Corresponding Authors: pederlh@stud.ntnu.no, kim.kristiansen@ntnu.no

In an effort to harvest energy from low-grade waste heat and the salinity gradient between sea- and fresh water, we investigated a possible concept combining the two energy sources. In conventional reverse electrodialysis (RED), the Gibbs energy of mixing between sea- and fresh water is exploited. However, a temperature difference may substantially improve the performance of the RED cell. We have previously shown this using water samples of brackish and seawater. Measurements with a test cell using real water samples from the Nidelven river and the fjord near Trondheim, Norway, yielded a Seebeck coefficient of 1.8 ± 0.1 mV/K 1 for the repeating unit cell in a RED power plant. With an ideal concentration potential of approximately 150 mV at constant temperature, the thermal driving force can give more than 1 % increase in cell potential per Kelvin of temperature difference. The effect of salt on these contributions to the potential have now been investigated for the four most abundant cations in sea water; Na^{+}, K^{+}, Mg^{2+} and Ca^{2+}. We have measured the thermoelectric effect using cation- exchange membranes and single-salt solutions of the respective chloride salts. The results show that the Seebeck can be related to the hydrated radius of the cation, which is not described before. The hydrated radius we used is a corrected stokes radius related to the viscocity of the solutions 2. This gives an empirical relation to predict the Seebeck effect in pure salt solutions, relevant for ions abundant in seawater.

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Compositional pore network model for gas condensate flow

Authors: Paula Reis[1]; Marcio Carvalho[1]

[1] *Pontifícia Universidade Católica do Rio de Janeiro*

Corresponding Authors: paulareis@lmmp.mec.puc-rio.br, msc@lmmp.mec.puc-rio.br

Hydrocarbon recovery from gas condensate reservoirs can be significantly reduced due to condensate blockage. As the dew point pressure of the reservoir fluid is reached, a liquid phase rich in heavy hydrocarbons condenses and builds up in the porous medium, reducing the availability of flowing paths for the gas. In order to assess the complex flow behavior of gas and condensate in porous media, a fully-implicit isothermal compositional pore network model is presented.
3D pore networks based on Micro-CT images of rocks represent porous media. Pore throats are described by capillaries with converging-diverging axisymmetric geometry that intersect at junctions with infinite conductance. Capillary conductances vary according to local phase saturations and capillary number, so that an alternation between annular flow and the accommodation of a stable liquid bridge in the capillary constriction is represented. A control volume is defined for every pore in the network, where the pressure and number of moles of each fluid component are calculated at every time step by solving a system of nonlinear conservation equations with Newton-Raphson method. Phase equilibrium calculations adopt a PT-flash with the Peng-Robinson EoS.
With the proposed model, relative permeability curves were generated and the compositional variation in the networks due to the difference in the gas and condensate mobilities was evaluated. The modeled relative permeability curves exhibited rate and IFT dependent behavior, as observed in curves obtained with coreflooding experiments. For the fluid mixture employed in the simulations, a switch from retrograde gas to volatile oil was observed, depending on the flow conditions.

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Fracture propagation in porous media during fluid injection

Author: Srutarshi Pradhan[1]

[1] *Researcher, PoreLab, NTNU, Trondheim, Norway*

Corresponding Author: srutarshi.pradhan@ntnu.no

Fluid injection operations 1 are regularly done in several field case scenarios like petroleum production, geothermal installation and underground CO2 storage. Normally fluids with high pressure are injected through the injection wells and sometimes fractures open-up at the well-boundaries. Although fractures are mostly seen as "disturbing elements"for the stability of wells and well-operations, in some cases fractures are "intended"-for example, in hydraulic fracturing scenario people create fractures to increase permeability (flow channels) in the porous rocks. Creation of optimal flow channels is also the main goal for geothermal power projects. However, fractures must be created in a controlled manner so that the well-integrity is not disturbed. Therefore, we need better understanding of physical processes that guide fracture propagation in porous media and we also need to develop tools for monitoring fracture propagation. Our lab experiments [2,3] show the stress-induced fracturing behavior of number of reservoir rocks during fluid injection scenarios. Using the acoustic emission (AE) monitoring system, we could track the major fracture propagation and micro-CT image analysis can show the fracture pattern inside the sample. In addition, we have developed a discrete element model (DEM) simulation code based on invasion percolation and distance dependent stress intensity factor (K) to mimic the stress-induced fracturing of reservoir rocks. Our

simulation code can take into account the presence of pre-existing fractures inside the sample. The simulation results agree qualitatively [4] with the experimental observations and such a numerical code can be used to study the entire parameter space with several important inputs like tensile strength distribution, breaking criteria, porosity, sample size, borehole pressure etc.

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4. Invited presentation on Fracture propagation during fluid injection: Experiment, modeling and monitoring towards field scale applications at "Fracmeet Conference", IMSc, Chennai, India in March 2019.

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Probing Chemical Interactions of Asphaltenes with Silica and Calcium Carbonate Surfaces

Author: Saleh Hassan[1]

Co-authors: Maxim Yutkin [2]; Sirisha Kamireddy [3]; Xiaozhen Hu [4]; Clayton Radke [5]; Tadeusz Patzek [2]

[1] *PhD Student - King Abdullah University of Science and Technology*

[2] *King Abdullah University of Science and Technology*

[3] *King Abdullah University of Science and Technology*

[4] *Key Laboratory of Thermo-Fluid Science and Engineering of Ministry of Education*

[5] *University of California, Berkeley*

Corresponding Authors: radke@berkeley.edu, jasonhu.xz@outlook.com, saleh.hassan@kaust.edu.sa, tadeusz.patzek@kaust.edu.sa, sirisha.kamireddy@kaust.edu.sa, maxim.yutkin@gmail.com

Understanding of crude oil interactions with mineral surfaces in the presence of thin water films is essential to optimize the enhanced oil recovery (EOR). Such interactions with minerals are strong, irreversible, and caused by complex asphaltenes that incorporate several chemical groups by stacking aromatic rings together. Asphaltenes are water-insoluble, bulky surface-active polar supermolecules. They congregate at the oil-brine interface defining oil interfacial properties through formation of gelatinous skins. Specifically, asphaltenes irreversibly deposited from the oil-brine interface onto reservoir mineral surfaces control rock wettability and, therefore, multi-phase capillary flow.

Studying crude oils or asphaltenes is difficult because of their varying composition, strong interfacial, and chemical activity. Sensitive analytical equipment is irreversibly contaminated by such substances. To overcome these issues, we split the problem into several parts. We study how different mono- and poly-functional groups mimic asphaltene interaction with mineral surfaces, like silica or calcium carbonate (CC).

Interaction of amino (cetrimonium-chloride, CTAC), carboxylate (sodium hexanoate/decanoate, NaHex), and sulphate (sodium-dodecyl-sulfate, NaDS) groups with silica and CC was studied on corresponding surfactants or oligomers using quartz crystal microbalance (QCM) [1-3].

The silica surface is negatively charged in brines with pH above 2. It attracts positively charged surfactants, like CTAC. However, the negatively charged surfactants, like NaHex or NaDS, hardly adsorb onto silica, even in the presence of calcium. In contrast to silica, CC surface has both positive and negative ion-exchange sites. Surfactant adsorption is brine and pH-dependent [4]. We found that CTAC adsorbs on CC in any brine composition. NaDS adsorbs onto CC surface only in the presence of calcium ions suggesting a contribution of an ion-bridging mechanism [5-7].

Adsorption of all studied surfactants is reversible and, consequently not representative of asphaltenes. Multi-functional compounds, like polymers, demonstrate irreversible adsorption like asphaltene. We studied adsorption of carbohydrates decorated with individual amines, sulphates, and carboxylates.

The carbohydrates with amine functional groups adsorb irreversibly on CC and silica in all tested brines with pH up to 10. High-molecular-weight amines (e.g., 90 kDa), cannot be desorbed easily. Therefore, crude oils with low base number (BN) make better candidates for EOR treatment. Unlike monomers, sulphonated or carboxylated polymers show adsorption, indicating enhancement of bridging mechanism in polymers. However, bridging is weaker than ion-exchange; therefore, we suggest that oils with high acid number (AN) and low BN would bind to rocks more weakly than oils with high BN and low AN.

These findings are important for designing chemically efficient detachment of asphaltenic oil from rock surface. Oils with high AN and low BN contain more carboxylic functional groups than amines, so weak bridging mechanism might be the main contributor for the oil attachment. In this case, flooding design should aim to disrupt bridging. No complete desorption or drastic wettability change is required. Weakening of the asphaltene interactions may lower requirement on water advancing contact angle just enough to induce spontaneous imbibition and thus increase efficiency of two-phase displacement. In conclusion, we suggest that oils with low BN are the best candidates for such EOR techniques, like low salinity waterflooding.

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Chemo-Hydro-Poromechanics of Enhanced Cracking in Geo-Energy Engineering

Author: ManMan Hu[1]

[1] *the University of Hong Kong*

Corresponding Author: mmhu@hku.hk

Chemo-Hydro-Poromechanics plays an essential role in the development of modern geo-energy engineering, including unconventional shale hydrocarbon recovery, enhanced geothermal systems, CO2 sequestration and utilization, Geological nuclear waste disposal. All of these developments require a sophisticated understanding of the coupling and feedbacks between the behavior of a porous geomaterial and the environment it is subject to, such as the temperature, chemical concentrations, mineral dissolution/precipitation, and other physical (or chemical) variables. This work aims to study the fundamentals of coupled chemo-hydro-mechanical processes in a porous geomaterial as encountered in typical scenarios of hydraulic fracturing, with a special emphasis on the role of the acidizing treatment.

In terms of modelling, how an individual crack propagates into a stressed medium subject to fluid pressure acting on the crack surfaces and meanwhile being affected by the chemically aggressive environment is a particularly interesting question. Subcritical crack propagation can be promoted by two means: 1) enhancing the stress localization in the vicinity of the crack tip, via e.g. decreasing the energy potential for generating new surfaces of micro-cracks; or 2) lowering the material toughness or damage tolerance (via e.g. chemical degradation induced by mass removal) in front of the crack tip. Acidizing treatment was invented for the latter purpose, but the induced coupled physio-chemical processes were found playing an important role on the local stress redistribution around the crack tip, as well as the evolution of the fracture energy release rate. A series of numerical experiments will be conducted using a multi-physics high-performance-computing finite-element simulator, REDBACK, specializing on dissipative rock mechanics problems based on the MOOSE environment. The emphasis of this study is placed on the feedback mechanisms between coupled processes of chemical softening by mineral mass removal, irreversible damage manifested as micro-cracking, micro-channeling induced alteration in local hydraulic conductivity and hence the delivery of acid, etc.

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Experimental study of particle deposition during immiscible displacement in a microchannel

Author: Ting Wu[1]

Co-authors: Zhibing Yang [1]; Yi-Feng Chen [1]; Ran Hu [1]

[1] *Wuhan University, School of Water Resources and Hydropower Engineering*

Corresponding Author: 2018202060075@whu.edu.cn

Immiscible displacement in porous media is an important process in a variety of natural and industrial settings, including water infiltration into soil, enhanced oil recovery, and microfluidics. While the effect of invading velocity and wettability on the pattern formation of immiscible displacement have been extensively studied, the fluid invasion dynamics in a suspension of solid particles in a liquid has received less attention. in which the aggregation of particles near the interface can significantly change the displacement process. Here we experimentally study the displacement of particle suspension by air in a microchannel. By varying the flow rate and the particle volume fraction in the suspension, we observed different particle deposition regimes ranging from no particle entrainment to particle monolayers within liquid films. We find that when the thickness of the entrained film of suspension is larger than the particle radius, it follows the Landau–Levich–Derjaguin law using the effective viscosity of the suspension. Moreover, by particle tracking, we have quantified the probability of particles entrained for various capillary numbers and particle volume fractions. The results show that the probability of particles near the invading front becoming entrained in the films increases with increasing capillary number.

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Interfacial Viscoelasticity in Crude Oil-water Systems

Author: Ahmed M. Saad[1]

Co-authors: Stefano Aime [2]; Sharath Mahavadi [3]; Y-Qiao Song [4]; Maxim Yutkin [5]; Tadeusz Patzek [1]; David A. Weitz [2]

[1] *KAUST*

[2] *Harvard University, USA*

[3] *Schlumberger-Doll Research, USA*

[4] *Massachusetts General Hospital*

[5] *King Abdullah University of Science and Technology*

Corresponding Authors: maxim.yutkin@gmail.com, ysong@slb.com, weitz@seas.harvard.edu, tadeusz.patzek@kaust.edu.sa, aime@seas.harvard.edu, ahmed.mohamedsaad@kaust.edu.sa, smahavadi@slb.com

Improved oil recovery from asphaltenic oil reservoirs may provide the world with a significant source of lower-cost energy over many decades. However, the mechanisms of how the surface active components in crude oil, such as asphaltenes, affect incremental oil production are still unclear [Yutkin et al. (2016)]. Experimentally, It has been shown that asphaltenes adsorb irreversibly at the crude oil/water interface [Freer et al. (2004), Mahavadi et al. (2008)] leading to the development of viscoelasticity [McLean et al. (1997)]. The effect of salinity of the aqueous phase on the interfacial viscoelasticity has been studied in 2D micro-models. It turns out that lower salinity brines lead to higher elasticity that eventually suppresses snap-off events, leading to higher oil recovery [Alvardo et al. (2014)]. The chemical composition of these interfacial films has been examined for crude oil/deionized (DI) water systems employing Fourier-Transform Infrared Spectroscopy (FTIR). The analysis revealed that the interface consists of different interfacial active species, including naphthenic acids [Andersen et al. (2017)].

In the current study, we varied the chemical composition of the aqueous phase to investigate how it affects absorption of different chemical species at the interface and its macroscopic properties. We combined shear and dilational rheology measurements with chemical analysis to inspect the evolution of the elastic modulus, surface tension, and changes in interfacial film composition. Our experiments covered a range of ionic compositions of the aqueous phase, from DI water to solutions of monovalent and divalent salts. The Interfacial shear rheology experiments were conducted using

a custom modification of the double-wall ring geometry to allow circulation of fluids along with changing the chemical composition. At the end of each experiment, the bulk crude oil is washed away by injecting fresh toluene to collect the interfacial film for FTIR analysis. To the best of our knowledge, this is the first setup that allows the measurement of shear interfacial properties with changing the chemical composition of the fluids while preserving the interfacial film undamaged. The effect of ionic composition on surface tension was investigated using dilational rheology experiments performed with the pulsating drop technique. Besides, this technique probes the extensional component of the surface elastic modulus.

Shear rheology data showed significant distinctions between different aqueous solutions in terms of the elastic modulus values and elasticity build-up dynamics. We believe that the initial period prior to the onset of elasticity is a regime dominated by molecular kinetics, with polar molecules arranging themselves on the interface. The chemical analysis of interfacial films formed during the above experiments demonstrated that the films are enriched with acidic polar species. We will also discuss how the film composition evolved with the change in water chemistry.

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Control of immiscible displacement patterns in disordered porous media

Authors: Xinlei Qi[None]; Zhengyuan Luo[None]; Bofeng Bai[None]

Corresponding Author: qixinlei@foxmail.com

Immiscible drainage in porous media plays an important role in many natural and industrial process, including enhanced oil recovery, CO2 sequestration1, water infiltration into soil2 and porous exchange columns. The displacement mechanism of immiscible fluid in porous media and the regulation of phase distribution are the key to solve these problems. The pore-scale structure of porous media has a decisive influence on the immiscible displacement process. Although some researchers have put forward several definitions of pore scale disordered structure[3-7], the effect of pore-scale structure disorder on the displacement process still has not been explored clearly[8]. In particular, the quantitative relationship between pore distribution disorder in porous media and displacement patterns (viscous fingering, capillary fingering and stable displacement) has not been established. Here, we study the impact of pore distribution disorder on immiscible drainage in disordered porous media with macroscopically constant porosity by means of high-resolution imaging in microfluidic flow cells. Our results suggest that the disorder of pore distribution act to displacement patterns for a predictable range of flow conditions. The study determined displacement parameters to get high

displacement efficiency for porous media with defined pore structure and provided design principles for porous materials with constant porosity.

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Remediation of solid wastes by nanosecond pulsed dielectric barrier discharge plasma

Author: Christos Aggelopoulos[1]

Co-author: Christos Tsakiroglou [2]

[1] *Foundation for Research and Technology Hellas, Institute of Chemical Engineering Sciences (FORTH/ICE-HT)*

[2] *Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT)*

Corresponding Authors: ctsakir@iceht.forth.gr, caggelop@iceht.forth.gr

Various technologies have been proposed to remediate industrial solid wastes such as incineration, solidification, biochemical processes and adsorption. Most of these technologies have low efficiency, slow kinetics, high-energy requirements and produce secondary pollution. Therefore, it is vital to explore and develop new solid waste remediation technologies that would be sustainable, efficient, rapid and cost-effective.
Over the last years, cold atmospheric plasma (CAP) technology has been applied as an advanced oxidation process (AOP) for the removal of organic pollutants from wastewater, polluted gas and contaminated soils 1. During CAP, the collisions between hot electrons of high energy and cold gas molecules can lead to the formation of highly reactive species such as excited atoms radicals, ions and ultraviolet photons through excitation, dissociation, ionization and recombination reactions. These species, due to their high oxidation potential, are very effective towards the fast oxidation and mineralization of organic pollutants. Therefore, CAP is considered as a very promising, green (no chemical reagents are required) and sustainable remediation technology of low energy cost/demands.
In this study, nanosecond pulsed dielectric barrier discharge (ns-DBD) was investigated as a CAP method for the regeneration of activated bauxite that has been used as adsorbent of lubricating oils and/or oils used in power transformers. The ns-DBD experiments were performed in a plane-to-grid reactor driven by nanosecond pulsed voltage supplied by means of a nanosecond pulse generator (NPG-18/3500). The generator can produce positive high-voltage pulses with amplitude regulated from 12 kV to 20 kV on matched 75 Ohm load (up to 25 kV on the DBD reactor in the present study). The pulse rise time was about 4 ns, the repetition rate up to 3.5 kHz and the maximum pulse energy

was 30 mJ. In the present study, voltage pulses of 20.8 kV and 24 kV at repetition rates (pulse frequencies) from 500 Hz to 2.5 kHz were examined. The effect of CAP operating conditions such as treatment time, applied voltage, energy efficiency, pulse frequency and air flow rate on total organic carbon (TOC) removal in contaminated bauxite was investigated. Furthermore, gas temperature was measured and a thorough exhaust gas analysis (CO, CO2, VOCs, etc.) was done. Finally, the main oil degradation intermediates were identified using Fourier Transform Infrared Spectroscopy (FTIR) and liquid chromatography-mass spectrometry (LC-MS).

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Efficient Simulation of Reactive Flow in Reservoirs Rocks at the Pore Scale

Authors: Christian Hinz[1]; Jens-Oliver Schwarz[1]; Andreas Weber[2]; Andreas Wiegmann[1]

[1] *Math2Market GmbH*

[2] *math2market*

Corresponding Authors: jens-oliver.schwarz@math2market.de, andreas.weber@math2market.de, andreas.wiegmann@math2marke
christian.hinz@math2market.de

Modelling of reactive flow in digital rocks requires the consideration of geochemistry and Digital Rock Physics (DRP) and relies on the assumption that the examined samples are representative for the properties of interest, which evolve during the simulation of 4D pore alteration. With the prerequisite of high image resolutions and large sample volumes, representative elementary volumes (REV) require numerically challenging domain sizes of 8.5 billion voxels (2048^3) and larger.

Here, we present a highly efficient approach to simulate reactive transport in REV domains based on the Lagrangian transport method. We apply mineral surface-related reaction rates to control the amount of kinetic pore alteration at locations determined by simulating advective and diffusive motion of virtual particles. The dynamic processing of particle-rock interactions allows the high performance required to handle large domains. Simulations at increased time step lengths consider an upscaling of kinetic precipitation and dissolution reactions to account for given mineral-specific reaction rates. We can thus simulate reactive flow at increased time scales.

We present reaction scenarios in typical reservoir rocks, such as the injection of hydrochloric acid into carbonate rock. The goal of this carbonate reservoir stimulation is to increase the permeability by enlarging the pore space. At equal reaction rate, different dissolution patterns develop in the rock, depending on the injection rate and the digital carbonate rock structure. These patterns can be predicted with reactive flow simulations. In them, the injection parameters leading to the most favorable dissolution of the reservoir rock and the correlated permeability increase are determined. In our approach, the reactive flow is modeled as a combined continuum/particle method by a combination of Python coding and the numerical code(s) in the DRP software GeoDict®.

In this ongoing project, numerical experiments qualitatively verify the numerical model. The model reproduces the dissolution patterns from the literature [1,2]. They correspond to the dissolution patterns: face dissolution, wormhole, uniform dissolution, and channeling. The formation of the patterns depends on the fluid velocity, reaction rate, and digital rock structure. We simulate on a carbonate sample from the Grosmont formation (Alberta, Canada) published in a DRP benchmark study [3].

The coupling of our highly efficient flow solver and particle transport simulation with a technically optimized workflow enables reactive transport simulations in sizable geometries at the pore scale. We aim to compare our results with time sequences of µCT-scans of real dissolution processes and offer a suitable tool for predicting the development of digital rock properties during continuous reactions at fluid-rock interfaces.

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Computational Multiscale Methods for Linear Poroelasticity using CEM-GMsFEM

Authors: Eric Chung[1]; Sai-Mang Pun[2]; Shubin Fu[1]; Robert Altmann[3]; Roland Maier[3]; Daniel Peterseim[3]

[1] *The Chinese University of Hong Kong*

[2] *Texas A&M University*

[3] *University of Augsburg*

Corresponding Authors: smpun@math.tamu.edu, tschung@math.cuhk.edu.hk

In this work, we employ the Constraint Energy Minimizing Generalized Multiscale Finite Element Method (CEM-GMsFEM) to solve the problem of linear heterogeneous poroelasticity with coefficients of high contrast. The proposed method makes use of the idea of energy minimization with suitable constraints in order to generate efficient basis functions for the displacement and the pressure. These basis functions are constructed by solving a class of local auxiliary optimization problems based on eigenfunctions containing local information on the heterogeneity. Techniques of oversampling are adapted to enhance the computational performance. The convergence of first order is shown and illustrated by a number of numerical tests.

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Measurement and Research of Two-phase Micro-force of Foam Fluid and Heavy Oil

Author: Zihan Gu[1]

Co-authors: Zhaomin Li [1]; Teng Lu [1]; Zhengxiao Xu [1]; Sheng Li [1]; Xinru Zhao [1]

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

Corresponding Authors: luteng@upc.edu.cn, 1052014043@qq.com, zzhaoxinru@163.com, 17854217153@163.com, lizhm@upc.edu.cn, b18020040@s.upc.edu.cn

Foam flooding technology is one of the common development methods to deal with heavy oil reservoirs.,However, the current research focus of foam flooding technology in China is mostly on the optimization and testing of macro-displacement effects,There are few studies on the micro-angle multiphase fluid displacement flow relationship, and the influence of various physical and chemical factors on such displacement phenomena. The influence of microscopic forces between fluids is one of the important parts.
This paper focuses on measuring and calculating the mechanism of mechanical forces between various heavy oils and foam fluids from a microscopic perspective, using a micro-camera device, and study the influence of related factors such as fluid viscosity. In this experimental study, two types of oil samples with different viscosities from oilfields were selected (121000mPa.s and 84400mPa.s respectively at room temperature and pressure), SDS surfactant solutions with a mass concentration of 2.5% and 5% were prepared as foaming agents for combined experiments. According to the analysis of the experimental results, it was found that at the 5% foaming agent concentration, the peak of the adsorption force between the oil sample with higher viscosity and foam was about 1.3 times that of the oil sample with lower viscosity; and at 2.5% foaming agent concentration, the viscosity The peak of the adsorption force between the larger oil sample and the foam is about 1.6 times of the smaller viscosity oil sample,In addition to the physical and chemical properties of crude oil, the properties of foaming agents are also important influencing factors that determine the forces between the phases of the multiphase fluid system, so further experimental verification is needed. In summary, the study of the micro-force interaction mechanism between foam fluids and heavy oils from a micro perspective will provide a certain theoretical basis for the further development of oilfield development technology and the further improvement of EOR technology for foam displacement heavy oils. With reference.

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Study on the distribution of micro remaining oil in different sedimentary microfacies by using glass etching displacement experiments

Author: xianbo luo[1]

[1] *CNOOC*

Corresponding Author: luoxb@cnooc.com.cn

according to the 1:1 conversion of the casting slice size of different sedimentary microfacies in P oilfield to the micro etched glass model, the micro residual oil distribution law of three different sedimentary microfacies was studied by the micro visual glass etch displacement experiment. The results show that the residual oil of the braided channel sedimentary microfacies mostly presents the obvious “network continuous” distribution, and the recovery factor is related to the oil washing efficiency When the injection volume reaches 30pv, the recovery rate is 55.3%, and the remaining oil is mainly in the form of continuous slices; when the injection volume reaches 15PV, the increase of sweep volume / displacement efficiency slows down gradually, and the sweep effect is good. As a whole, the remaining oil has a stable recovery rate in the dead oil area At about 60%, the remaining oil after water flooding mainly exists in the form of continuous sheet, oil drop and oil film, among which the most is in the form of continuous sheet and oil drop, and the least is in the form of oil film; the point bar sedimentary microfacies, with the increase of injection multiple, lead to the

spread gradually extending to the far end, the residual oil saturation decreases, and there is an island like residual oil area as a whole when the injection volume reaches 7PV After that, the increase of sweep volume / displacement efficiency slowed down gradually, and the recovery rate was only 35%. After water flooding, the remaining oil was mainly in the form of continuous sheet and oil drop. The experimental results can guide the next potential tapping direction of P oilfield. The swept coefficient of the core beach is high, but the proportion of oil drop and oil film remaining oil in the affected area is high. In the later stage, the main potential tapping direction is to improve the oil displacement efficiency. In the area affected by the braided river channel, the oil washing efficiency is high. In the later stage, the main potential tapping direction is to improve the swept coefficient. The edge beach sweep is poor, and it is easy to local outburst in the early stage In the later stage, the main direction is to strengthen the profile adjustment.

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Study on Fluid Extraction Considering Reservoir Microstructure

Author: Zhou Fang[1]

Co-authors: Jifeng Qu ; Caiqi Zhang ; Lei Zhang ; Guangming Pan

[1] *Research Institute, CNOOC*

Corresponding Author: fangzhou2@cnooc.com.cn

By comparing the development of several water-injection oilfields in the Shijiutuo Uplift of Bohai Oilfield, it is found that fluvial oilfields under the same high-porosity and high-permeability reservoir conditions there have significant differences such as Qinhuangdao 32-6 oilfield and Nanpu 35-2 oilfield in dimensionless fluid recovery index and fluid recovery rate.

The dimensionless fluid recovery index and fluid recovery rate of Minghuazhen Formation represented by Qinhuangdao 32-6 oilfield were high, but Nanpu 35-2 oilfield were quite low. Aiming at this problem, a research on the influence of the reservoir microstructure on the development effect has been carried out, and combined with the petrological and mineralogical analysis of the core and the scanning electron microscopy results, it discovered that the difference in reservoir microstructure affected the development effect of the oil field.

The clay minerals and heterogeneous particles contained in the reservoir have potential water sensitivity and particle migration damage. In the process of oilfield waterflooding development, the expansive clay in the reservoir swells with the injected water, causing water sensitivity damage, resulting in a decrease in formation permeability.

Through research, the main control factors restricting the fluid extraction in Nanpu 35-2 oilfield were clearly defined. Based on the analysis results of water sensitivity experiments in Nanbao 35-2 oilfield, the quantitative characterization of water permeability damage to reservoir permeability was established.

By considering the influence of water sensitivity on the phase permeability curve, a water sensitivity factor was introduced to correct the phase permeability curve of Nanpu 35-2 oil field, and the dimensionless fluid recovery index curve was obtained after considering water sensitivity damage.

In the current state of waterflooding development, a method for correcting the reasonable fluid production of Nanpu 35-2 oilfield is proposed by fitting the actual oilfield conditions.

The determination of the additional pressure difference due to the limited sensitivity of the liquid volume due to water sensitivity has resulted in the optimized liquid extraction guidance for the

Nanpu 35-2 oilfield under the additional pressure difference.

Based on the optimized phase permeability simulation, the upper limit of reasonable production pressure difference of Nanpu 35-2 oilfield considering the reservoir microstructure is 7.5MPa, and the daily liquid production range is between 400 ~ 700 cubic meters. Three production wells in Nanpu 35-2 oilfield were selected for simulation and field tests. By continuing to enlarge the pressure differential to about 6MPa, the average daily oil production of oil wells increased by 60%, and the production fluid of one well rose from 110 cubic meters to 480 cubic meters The daily output of oil increased by 10 cubic meters.

With well performed pilot test, in the future, this guidance model can be used as the basis for the design on subsequent fluid extraction strategies of fluvial oilfields.

Keywords: Fluvial oilfields, Reservoir microcosm, Water sensitivity factor, Correction of permeability curve, Additional pressure difference

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Wastewater treatment in continuous-flow fixed-bed photoreactors packed with ZnO nanoparticles-coated beads

Author: Christos Tsakiroglou[1]

Co-authors: Michalis Karavasilis [2]; Christos Aggelopoulos [3]

[1] *Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT)*

[2] *Foundation for Reserach and Technology Hellas - Institute of Chemical Engineering Sciences and Department of Chemistry, University of Patras*

[3] *FORTH/ICE-HT*

Corresponding Authors: mkaravas@iceht.forth.gr, caggelop@iceht.forth.gr, ctsakir@iceht.forth.gr

In spite of the progress achieved on the photo-catalysis during the last 20 years, particularly with reference to the development of nanocomposite materials for the destruction of a great variety of recalcitrant contaminants in water streams, there is still a gap of knowledge on the optimization of the performance of continuous-flow photo-reactors [1,2]. Zinc-oxide (ZnO) nanoparticles were immobilized on Duranit (80% silica+ 20% alumina) inert balls, by immersing them in aqueous solution of zinc acetate dehydrate (ZnAc) under stirring at 80oC for 30 min, separating the spheres from the solution, and calcinating them in an oven at 450oC for 2 hrs. Complete characterization of the ZnO nanoparticles, substrate surface, and substrate-coated ZnO was done by a variety of techniques (e.g. TEM, SEM, BET, XRD, FT-IR). The photocatalytic performance of immobilized ZnO was assessed with a parametric study of Phenol (Ph) degradation in batch photo-reactors, using as light source UV-lamps of nominal power 6 W / 22 W and emission peak at 365 nm. To estimate the reaction kinetics, the residual Ph concentration was measured as a function of time with UV-Vis spectroscopy. Continuous flow tests of photocatalysis were conducted in fixed-bed annular photoreactors, packed with ZnO-coated beads, and illuminated with a UV lamp (8 W / 365 nm) placed along its center line. With the aid of a peristaltic pump, the Ph solution was recycled between the reactor, and a continuously-stirred vessel, where the solution pH and redox potential were monitored. A one-dimensional dynamic mathematical model of the operation of the continuous flow system was developed by coupling the mass-transfer with reactive processes. The model was used to: (i) estimate the kinetic parameters of photocatalytic reactions by fitting its numerical solution to transient experimental measurements; (ii) design flow-through experiments; (iii) scale-up the process to a pilot unit.

ACKNOWLEDGMENTS
This work was implemented under the Action "Promotion of Transnational Research Projects for Small and Medium Size Enterprises"and is co-financed by the European Union and National Resources through the Operational Program "Western Greece 2014-2020"*(project title: "Design, optimization and construction of an energy-autonomous photocatalytic unit for the on-site remediation of wastewater-PHOTOWATER"; project code: MIS 5032954).*

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Study on water injection mechanism of tight reservoir based on large-scale outcrop physical simulation experiment

Authors: Yutian Luo[None]; Xuewei Liu[None]

Co-authors: zhengming yang [1]; Xiangui Liu [2]; guozhong Liu ; Xinlin Zhao

[1] *PetroChina Research Institute of Petroleum Exploration & Development*

[2] *Research Institute of Petroleum Exploration & Development, China National Petroleum Corporation*

Corresponding Authors: yzhm69@petrochina.com.cn, luoyutian@petrochina.com.cn, liuxiangui69@petrochina.com.cn, lxw69@petrochina.com.cn, lgz1027@petrochina.com.cn

Tight reservoirs have extremely low permeability and porosity, complex pore structures, and unclear oil-water distribution mechanisms. Small core experiments are difficult to find the water flooding front and the rest oil. This paper uses a large-scale outcrop physical simulation experiment system to simulate the water flooding development process under different conditions. It is found that the Jamin effect is the main factor forming the water flooding resistance. The experiment takes the tight reservoirs of the Ordos Basin as the research object. Through experiments, it is found that there is a large pressure drop in the oil-water transition zone of the water flooding front, and the liquid production is faster in the initial stage of production. In the first 1/3 of the time, 80% of the liquid volume and 90% of the oil volume were produced. The anhydrous recovery rate was 17%, and the recovery rate after producing water was 5%. By comparing models of different fracturing scales, it is found that fractures can effectively improve oil recovery speed and recovery rate, fracturing oil production wells can increase oil production rate by 2 times, oil and water well fracturing can increase oil production rate by 3 times, and recovery rate after fracturing can be improved About 12%.

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Discrete Multiple Media Geological Modelling Method

Authors: Jiaxin Dong[None]; Qiquan Ran[None]; Wen Shi[None]

Corresponding Author: 672741310@qq.com

The pores in unconventional tight reservoirs are smaller, with nano-nano/micro-micro scale pore media at different scales. The composition and quantity distribution patterns of pores at different scales are quite different. Moreover, pores at different scales show discrete discontinuous distribution in space. The spatial distribution patterns are quite different. The geometric and physical parameters of pore media at different scales are quite different. At the same time, natural/hydraulic micro-nano scale fractures also exist in tight reservoirs. These micro-nano scale fractures are of large quantity and small sizes, which cannot be treated as deterministic discrete fractures. But on the microscopic scale they still have certain storage capacity and flow capability to communicate pores of different scales. In addition, they show discrete and discontinuous distribution in space. Therefore, the pores and micro-nano fractures at different scales are regarded as discretely distributed micro scale discrete media. The spatial distribution and quantity distribution of pores and fractures at different scales are used as constraints to generate discrete multiple media. It is a leap forward for the continuous modeling method of the property parameters of a single type pore media. The modeling technique of the property parameters for discontinuous discrete multiple media has been established.
The steps are as follows. ①According to the macroscopic heterogeneity for spatial distribution of such geological conditions as lithology, lithofacies, reservoir types, degree and scales of natural fractures, magnitude and direction of ground stress, and fluid properties, the first level regions are partitioned with macroscopic large-scale heterogeneity. ②According to the differences in small-scale geological conditions and heterogeneity within the same region, it is partitioned into several second level representative elements. According to the distribution characteristics of different representative elements, a suitable unstructured grid is used to partition this area, which forms the first level discrete grids that correspond to representative elements③Within a representative element, the third levels of multiple media are partitioned according to the quantity and spatial distribution of microscopic pores and fractures at different scales. The number of medium types of multiple media are decided according to the quantitative distribution and the volume percentage of multiple media at different scales. According to the spatial distribution law of multiple media at different scales, they are divided into two kinds of multiple media modes: nested distribution type media and randomly interacting distribution type media. By selecting appropriate unstructured grids, representative elements are discretized into nested and interactive second level grids. Moreover, discrete multiple media grids and discrete multiple media are generated accordingly. Using the discrete multiple media modeling methods, we establish the geometric parameters (pore/pore throat radius, etc.), property parameters (porosity and permeability, etc.), flow parameters and other modes of the discrete multiple media. Eventually, the discrete multiple media geological model is generated.

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A Numerical Model for Enzymatically Induced Calcite Precipitation

Authors: Johannes Hommel[1]; Arda Akyel[2]; Adrienne Phillips[3]; Robin Gerlach[3]; Al Cunningham[4]; Holger Class[1]

[1] *University of Stuttgart*

[2] *Ph.D. Student*

[3] *Montana State University*

[4] *Center for Biofilm Engineering, Montana State University*

Corresponding Authors: holger.class@iws.uni-stuttgart.de, johannes.hommel@iws.uni-stuttgart.de, arda.akyel@montana.edu, adrienne.phillips@montana.edu, al_c@montana.edu, robin_g@montana.edu

One of the key issues of underground gas storage is the long-term security of the storage site. Amongst the different storage mechanisms, cap-rock integrity is crucial for preventing leakage of the stored gas due to buoyancy into shallower aquifers or, ultimately, the atmosphere. This leakage would reduce the efficiency of underground gas storage and pose a threat to the environment. Ureolysis-driven, microbially induced calcite precipitation (MICP) has been proven to be an effective technology to mitigate potential leakage by sealing high-permeability zones in cap rocks or well defects.

A similar emerging biomineralization method is enzymatically induced calcium carbonate precipitation (EICP). EICP is advantageous to MICP as the enzyme is still active at conditions, where the commonly used microbe Sporosarcina pasteurii will cease to be active. This expands the applicability of biomineralization to higher temperatures enabling its use in leakage mitigation deeper in the subsurface than previously possible. Additionally, since heat inactivates the cells, but the enzyme is still active up to higher temperatures, any application of MICP at such high-temperature conditions will automatically transition into an EICP application.

A new conceptual and numerical model for EICP is presented. The model has been calibrated and validated using quasi-1D column experiments designed to provide the necessary data for model calibration. The challenge is constructing a predictive model for concerted permeability reduction in the underground with EICP is to quantify the complex interaction between flow, transport,adsorbed enzyme growth, and reaction kinetics.

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Experimental Methods and Imaging for Enzymatically Induced Calcite Precipitation in micro-fluidic devices

Author: Felix Weinhardt[None]

Co-authors: Johannes Hommel [1]; Robin Gerlach [2]; Nikolaos Karadimitriou [3]; Holger Steeb [1]; Holger Class ; Dongwon Lee ; Samaneh Vahid Dastjerdi

[1] *University of Stuttgart*

[2] *Montana State University*

[3] *Institute of Mechanics (CE), Stuttgart University*

Corresponding Authors: johannes.hommel@iws.uni-stuttgart.de, nikos.karadimitriou@mechbau.uni-stuttgart.de, felix.weinhardt@iws.uni-stuttgart.de, robin_g@montana.edu, holger.steeb@mechbau.uni-stuttgart.de

Enzymatically Induced Calcite Precipitation (EICP) in porous media can be used as an engineering option to achieve targeted precipitation in the pore space. 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 conventional porosity-permeability relations 1. To improve REV-scale models, we investigate the effect of EICP on hydraulic properties in micro-fluidic experiments, measuring the pressure drop to calculate the permeability while quantifying the change in porosity by optical microscopy as well as X-Ray Computed Tomography (XRCT). The results of the study show the enormous benefits and insights of combining both microscopy and XRCT with hydraulic measurements in micro-fluidic devices. This allows for a quantitative analysis of the evolution of precipitates while monitoring the influence on the permeability, and thus improves the interpretation of monitored flow data dependent on changes in pore morphology.

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A multilayer model for reactive flow in fractured porous media

Authors: Alessio Fumagalli[1]; Anna Scotti[1]; Luca Formaggia[1]

[1] *Politecnico di Milano*

Corresponding Authors: luca.formaggia@polimi.it, anna.scotti@polimi.it

The presence of fractures has an impact on subsurface flows at all scales: flow tends to focus along highly permeable fractures, which can create "shortcuts" in the domain, or, in the case of cemented fractures, we have low permeability barriers in the domain. In the context of reactive transport fractures can be responsible for fast transport of fluid with different chemical composition with respect to the surrounding matrix: this occurs for instance in geothermal reservoirs where water with different salinity, solutes and temperature is injected in the subsurface. This differences in composition and temperature can trigger transformations such as mineral precipitation, dissolution or replacement, with an impact on porosity and fracture aperture. We propose a model to account explicitly for the presence of fractures and their impact on the flow, transport and reactions. We rely on a geometrically reduced model where fractures can be represented by surfaces or lines coupled with the surrounding porous medium. Moreover, we want to account for the fact that, depending on the speed of the reactions relative to the flow velocity, we can observe a thin layer around fractures where most of the geochemical phenomena are concentrated. This layer is in turn represented as a surface with variable-in-time thickness coupled on one side with the fracture "core", on the other with the bulk porous medium. The equations describing flow and transport are thus a coupled of mixed-dimensional PDEs approximated by means of lowest order mixed finite elements, 1. We will consider a simple model for mineral precipitation dissolution following 2. To avoid the occurrence of negative concentrations and oscillations when the amount of precipitate approaches zero we adopt an event location strategy to detect the discontinuity in the ODE describing the reaction part, which is, for this reason, split from advection and diffusion by means of a first-order operator splitting.

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Pore Scale Mechanisms of Chemical Injection into Heterogeneous Micromodel

Authors: Dongqing Cao[1]; Ming Han[1]; Jinxun Wang[2]; Abdulkareem AlSofi[2]

[1] *Aramco Asia*
[2] *Saudi Aramco*

Corresponding Author: dongqing.cao@aramcoasia.com

Chemical injection such as surfactant and polymer has been extensively applied in the oilfield.At pore scale, the chemical injection involves complicated chemical/oil/rock interactions especially in heterogeneous reservoir, which may be overlooked in the macroscopic description like mobility ratio and capillary number. This study investigates the pore scale mechanisms of polymer and surfactant flows through the visible heterogeneous micromodel.
The etched glass micromodel was used with a 4cm*4cm pore network from a core slice image of the nature carbonate core plug. The micromodel was treated to oil-wet by crude oil. An amphoteric surfactant and a sulfonated polymer was selected for the micromodel tests. The chemical was injected into the oil saturated micromodel following a water injection. The oil production and real-time flow image were collected. The flow rate ranged from 0.001 to 0.005 ml/min and the injection volume varied from 1 to 2 pore volume.
The oil production of different injection scenarios was compared. With the selected surfactant/polymer formulation, more chemical injection at median flow rate 0.0025ml/min produced the more oil. Surfactant and polymer co-injection had much higher oil production than the individual injection. At pore scale,the waterflood tended to invade the large pores and bypass oil in the small pores, dead end pores and the pores in the low permeability area. In the chemical injection, the residual oil was mainly triggered by the low capillary force caused by the ultra-low interfacial tension. Wettability hysteresis made the remobilization more difficult. Sufficient time rather than high flow rate was necessary for chemical to touch with the remaining oil. The polymer only could hardly trigger the oil blobs. The moving oil was stretched into oil membrane attaching on the walls due to the oil-wet nature. The membrane moved forward when there was effective tangential stress on the water oil interface, as in the polymer flooding. The surfactant only could not generate sufficient moving rate to produce the oil. Free oil droplet snapped-off from the oil membrane helped the oil moving. The large oil blob in the low permeability area contributed much of the oil production due to a continuous oil flow path extended to the outlet.
The work provides the new insights of chemical injections into the heterogeneous reservoir, which improves the understanding in the application of chemical related production methods.

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Experimental Study on Two-phase Miscible Displacement Pattern of Porous Media

Authors: Wei Guo[1]; Ran Hu[1]

[1] *Wuhan University*

Corresponding Authors: 243880812@qq.com, 976014475@qq.com

Viscous fingering occurs when a less viscous fluid displaces a more viscous fluid. Here we design a microfluidic-visualization system to perform the displacement of two miscible fluids. Experiments of water displacing glycerol are conducted at five flow rates (0.05~5μL/min), four viscosity ratios (50~1000). We observe a series of nonlinear finger interactions including spreading, shielding, coalescence and even tip-splitting. We find that there are two main mechanisms controlling the displacements. The displacements are initially dominated by diffusion. But later convection dominates flow and induces a large range of fingers, which results in significant variation of the mixing length, the averaged one-dimensional axial concentration profile and the concentration of the displacing phase. We further discover that the transition between diffusion and convection seems to be sensitive to the Peclet number (Pe) and viscosity ratio (M). When flow rate reaches the maximum (5ul/min), the flow is mainly dominated by convection which results in severe viscous fingering. Larger viscosity ratio seems to induce fingering more easily.

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Research on Different Storage Space Types of Marine Carbonate Buried Hills and Their Impact on Liquid Production Capacity——A case from the X structure of Shijiutuo uplift in Bohai Bay Basin

Author: Peng Shi[1]

Co-authors: Yong Hu ; Caiqi Zhang ; Zhou Fang ; Guangming Pan

[1] *Research Institute, CNOOC*

Corresponding Author: shipeng7@cnooc.com.cn

Carbonate buried hill is a significant oil and gas reservoir system in the world, of which the fluid production capacity and production characteristics of different types of storage spaces are quite different. There are few buried hill oilfields in the Bohai Sea, equally few studies on buried hill storage space and fluid production capacity. The X structure buried hill of the Shijiutuo uplift in the Bohai bay is an Ordovician carbonate buried hill, the reservoir rocks are mainly siliceous dolomite and siliceous limestone; reservoir spaces include intercrystalline pores, dissolution pores, dissolution fractures, and structural fractures; with undeveloped primary joint fractures and karst caves. The test production of 10 exploratory wells shows extremely different results which the daily fluid production levels which range from 0 to 1,310 tons. In order to clarify the storage space types of different carbonate buried hills and their fluid production capacity, the research is conducted based on core, test, slice, analysis and other data.

The result shows:

(1) Three types of storage space:
Type I develops high-angle structural fractures. The fractures are long and wide and unfilled, with a daily production of 1,310 tons;
Type II develops secondary structural fractures, dissolution pores and dissolution fractures. Local cracks are filled with calcite or semi-filled with organic matter, the phenomenon of oil immersion is visible, with a daily output of 200 ~ 350 tons;
Type III is subjected to diagenesis such as late compaction and filling, so that the fractures and dissolved pores formed in the early stage are filled, or the pores are isolated, therefore the reservoir heterogeneity is enhanced, with a daily production less than 30 tons.

(2) Reservoir type of Type I is with fractures connected to each other which have strong reservoir, seepage capacity and strong fluid production capacity;
Type II dissolution holes are the main storage space, and the semi-filled secondary fractures have good seepage ability and medium fluid production capacity;
Type III, due to serious filling, connectivity of holes and joints is poor, together with poor seepage ability and weak fluid production ability.

This study has certain significance for exploring the liquid production capacity of different types of reservoir structures of offshore limestone buried hill reservoirs.

Key words: Carbonate buried hill; Storage space; Test production; Production capacity; Bohai Bay Basin.

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Permeation and separation of CH4/CO2, N2/O2 mixtures through single-layer nanoporous graphene membranes : theory and molecular simulations.

Authors: Juncheng Guo[1]; Romain Vermorel[2]; Guillaume Galliero[3]

[1] *LFCR, E2S-UPPA, University of Pau and Pays de l'Adour*

[2] *LFCR, E2S-UPPA*

[3] *Université de Pau et des Pays de l'Adour, France*

Corresponding Authors: romain.vermorel@univ-pau.fr, juncheng.guo@etud.univ-pau.fr, guillaume.galliero@univ-pau.fr

Nanoporous graphene membranes are gaining attention in the field of water desalination 1 and gas separation 2. In the field of gas separation, perm-selective membranes technology consumes less energy than other conventional technologies. Due to nanoporous graphene's atomic thickness and controllable pore size in molecular diameter, it is considered as the most favorable membrane material showing a high selectivity. For instance, in the context of natural gas production and air separation, the separation of CH4/CO2, N2/O2 mixtures would greatly benefit from these new materials. With the rapid development in graphene fabrication technology, breakthroughs in nanoporous graphene membranes are expected in the next few years and quite sufficient data can be found in publications. However, there is no accurate theory with which we can predict gas permeation and separation factor quantitively.

In most researches, analytical frameworks are expressed using Arrhenius-type equations which assume activated diffusion is the only permeation mechanism. Nevertheless, recent work from our group [3] shows that Arrhenius-type equations are too simple to predict the diffusive transport coefficient correctly. The authors performed molecular dynamics simulations on a simplified model of single-layer porous membranes. They found that the transport coefficient is related to a well-defined accessible porosity and a thermodynamic factor, which can be computed from the potential of mean force (PMF) between the membrane atoms and the permeating gas molecules. Simulated transport coefficients are in good agreement with the predictions of this theory.

In this work, we show how to extend and apply this theoretical model to more realistic molecular models of nanoporous graphene membranes. By means of Equilibrium (EMD) and Non Equilibrium (NEMD) molecular dynamics simulations, we explore the permeation and separation of CH4/CO2, N2/O2 mixtures through porous graphenes exhibiting different pore sizes and geometry. Furthermore, we investigate the effect of thermodynamic conditions (pressure, temperature, mixture composition) on the diffusive transport coefficients. We will report our latest results and compare simulation data to the extended theoretical model.

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Study on the coupling mathematical model of gas-water two-phase seepage and wellbore pipe flow in fractured horizontal Wells in volcanic gas reservoirs

Author: Cheng Fu[1]

Co-authors: Tianyue Guo [1]; Bin Huang [1]; Tingting Zhu [1]

[1] *Northeast Petroleum University*

Corresponding Authors: huangbin111@163.com, cheng_fu111@163.com, yueyuepikaqiu@163.com, ztt950618@163.com

The volcanic gas reservoir of Xushen gas field is the main production layer of natural gas development in Daqing reservoir in the future. Although this kind of gas reservoir is rich in resources, it is difficult to develop because of its poor physical property and complicated seepage mechanism. Most of the gas wells are fractured horizontal wells, with low single well production, small well control dynamic reserves, water layer generally developed at the bottom, and low stable production capacity of gas Wells. Therefore, it is of great significance to study the gas-water two-phase productivity of fractured horizontal Wells in volcanic gas reservoirs.
Based on the principle of gas-water two-phase seepage and the non-linear seepage mechanism of gas reservoir, according to the principle of equal flow rate and momentum theorem, combined with the nature of gas and the actual gas state equation, taking into account the internal friction pressure drop of wellbore, acceleration pressure drop and ball seat pressure drop, this paper establishes a matrix-natural fracture-artificial fracture-wellbore volcanic gas reservoir fractured horizontal well gas-water two-phase seepage and wellbore pipe flow coupling mathematical model, and solves the model by VB programming. The productivity and pressure distribution are predicted. At the same time, the influencing factors of gas-water two-phase productivity of fractured horizontal wells in volcanic gas reservoirs are studied. It is found that the degree of influence of stress sensitivity coefficients of different media on productivity is natural fracture or secondary fracture stress sensitivity coefficient, artificial main fracture stress sensitivity coefficient and matrix stress sensitivity coefficient from large to small. The high-speed nonlinear coefficient has great influence on the productivity, while the starting pressure gradient has little influence on the productivity. Finally, the accuracy of the model is verified by using the production data of five existing horizontal wells, with an average accuracy of 90.28%. The results show that the research results in this paper have certain reference significance for productivity prediction of fractured horizontal wells in low permeability volcanic gas reservoirs.

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Direct imaging of bubble ripening in two-dimensional porous media micromodels

Authors: Nerine Joewondo[1]; Valeria Garbin[2]; Ronny Pini[1]

[1] *Imperial College London*

[2] *Delft University of Technology*

Corresponding Authors: nj18@ic.ac.uk, v.garbin@tudelft.nl, r.pini@imperial.ac.uk

The subsurface storage potential of CO_2 is largely dominated by capillary action that generates a so-called residual phase in the pores of the rock in the form of disconnected bubbles 1. Understanding the temporal and spatial evolution of this residual phase is key to ensure the long-term storage security of CO_2.
A single spherical gas bubble suspended in a liquid either dissolves or grows depending on the saturation of the liquid surrounding the gas phase. The dynamics of the process are controlled by the interplay between the diffusive mass transport and the Laplace pressure, which is inversely proportional to the bubble radius. When multiple bubbles are present, Ostwald ripening can occur, a process where large bubbles grow at the expense of smaller ones, as a result of the difference in Laplace pressure between the bubbles.
Confinement within a porous medium complicates considerably this picture by constraining the physical growth of the bubble, in addition to limiting diffusive mass transport. A gas bubble can in fact expand beyond the limits of the pore body into the adjacent pore-throats; under these conditions, the controlling Laplace pressure is determined by the local interface curvature within the (small) pore-throats, rather than by the size of the bubble itself 2. The analysis and experimental evidence of the evolution of a bubble population in a porous medium have been so-far quite limited.
To understand the factors affecting the stability of residually trapped CO_2, we observe the interactions of a population of air bubbles surrounded by undersaturated water in a 2D porous medium micromodel in isothermal conditions. An image processing routine was developed to extract the temporal evolution of size, local and mean curvatures of each bubble throughout its lifetime. We observe: i) ripening that is characterised by the decrease of number of bubbles and the narrowing of the distribution of local curvatures over time; ii) dissolution and disappearance of bubbles smaller than the pore throat diameter; and iii) the onset time of mass transfer between neighbouring bubbles to be in the order of ~10 times the bulk diffusive timescale. The experiments also reveal the local shape evolution of each bubble in response to its growth or dissolution. During this process, one or more interfaces either retract out of or advance into a pore throat. Notably, the moving interface is not necessarily the interface closest to an interface of a neighbouring bubble.

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Curvature Correction to Model Capillary Driven Flows at the Pore-Scale Using Volume-of-Fluid

Authors: Saideep Pavuluri[1]; Julien Maes[1]; Florian Doster[None]

[1] *Heriot-Watt University*

Corresponding Authors: f.doster@hw.ac.uk, saideep.pavuluri@pet.hw.ac.uk, j.maes@hw.ac.uk

Curvature Correction to Model Capillary Driven Flows at the Pore-Scale Using Volume-of-Fluid
Saideep Pavuluri*,1, Julien Maes2, Florian Doster2
1 –Bureau de Recherches Géologiques et Minières (BRGM), Orléans, France
2 –Energy Geosciences Infrastructure Society, Heriot-Watt University, Edinburgh, UK

Using direct numerical simulations (DNS) to accurately model capillary driven flows is a challenge primarily caused due to the difficulty in approximating capillary forces. In order to calculate capillary forces, interfacial curvature has to be calculated. We show by proposing a benchmark case-study and testing various volume of fluid (VOF) formulations that the calculation of the interfacial curvature can be critical with respect to even qualitative behaviour.
In this study, we investigate spontaneous imbibition in a pore singlet where the transition zone shapes vary. Based on the considered fluid and solid properties, capillary barriers may occur 1. We compare the precision of various VOF formulations namely, the continuum surface force (CSF) 2, the smooth surface force (CSF-Sm) [3], the sharp surface force (SSF) [3] and the filtered surface force (FSF) [3] for the proposed benchmark study.
We notice that the conventional expression used to compute the interfacial curvature is not accurate considering the above mentioned VOF formulations especially when dealing with unstructured meshes which are a prerequisite to capture the shape of pores. We identify a curvature correction without which all the above mentioned formulations fail to obtain physically expected results. For this benchmark study, after considering the proposed curvature correction, we notice that smoothing the VOF's colour function and filtering capillary terms must be done with care else might result in erroneous prediction of the fluids displacement. On the other hand, CSF and applying a minimal sharpening to the VOF's colour function are seen to closely match the expected solution of contact angle at which spontaneous imbibition occurs.
We further investigate the pore filling event using the above mentioned formulations considering the curvature correction when inertial effects are not negligible.

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Nondestructive high-throughput screening of nanopore geometry in porous membranes by imbibition: Laser-Interferometry and Dilatometry Experiments

Authors: Juan Sanchez Calzado[1]; Zhuoqing Li[1]; Luisa G. Cencha[2]; Michael Kappl[3]; Floudas George [3]; Claudio L.A. Berli[4]; Steinhart Martin[5]; Michael Fröba[6]; Raul Urteaga[2]; Patrick Huber[1]

[1] *Hamburg University of Technology*

[2] *IFIS-Litoral (Universidad Nacional del Litoral-CONICET), Guemes 3450, 3000 Santa Fe, Argentina*

[3] *Max Planck Institute for Polymer Research, D-55128 Mainz, Germany*

[4] *INTEC (Universidad Nacional del Litoral-CONICET), Predio CCT CONICET Santa Fe, RN 168, 3000 Santa Fe, Argentina*

[5] *Institut fu€r Chemie neuer Materialien, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany*

[6] *University of Hamburg*

Corresponding Authors: patrick.huber@tuhh.de, froeba@chemie.uni-hamburg.de, zhuoqing.li@tuhh.de, juan.sanchez@tuhh.de

Nanoporous media, in particular, monolithic porous membranes play an increasing scientific and technological role. Among the applications of porous membranes stand out filtration and separation processes, the study of confinement effects in soft matter, and energy harvesting. However, their characterization in terms of pore size and pore homogeneity is still an extremely demanding experimental task, even though it is of crucial importance for the interpretation of experiments and for the understanding of functional performance of nanoporous membranes. The sample requirements for the most prominent characterization methods of nanoporous materials, such as volumetric sorption isotherm measurements, mercury porosimetry, and electron microscopy, necessitate powders or small sample pieces and thus a destruction of the porous medium. Here, we present a theoretical analysis showing that simple, capillarity-driven filling experiments allow one to nondestructively analyze the pore geometry of macroscopic porous membranes with nanoscale spatial resolution in terms of pore diameter (gradients) 1. Moreover, we validate this method by experiments on the imbibition dynamics of several selected simple liquids in archetypical monolithic nanoporous media, i.e., anodic aluminum oxide (AAO) membranes. Additionally, we present dilatometry experiments on imbibition-induced deformation dynamics for water in nanoporous carbon, silica and polymers. These experiments document a competition of surface-stress and Laplace pressure contributions during the imbibition process [2,3,4] that also allows us to infer information on the pore size of monolithic nanoporous solids.

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Multi-Scale Benchmarking of a Coupled Geochemical Transport Solver

Authors: Saideep Pavuluri[1]; Christophe Tournassat[2]; Francis Claret[2]; Cyprien Soulaine[3]

[1] *Heriot-Watt University*

[2] *Bureau de Recherches Géologiques et Minières (BRGM)*

[3] *Stanford University*

Corresponding Authors: cyprien.soulaine@gmail.com, c.tournassat@brgm.fr, saideep.pavuluri@pet.hw.ac.uk, f.claret@brgm.fr

We developed an integrated open-source simulator to model hydro-geochemical processes at various scales of interest which include the pore-scale, an intermediate (hybrid) scale and the reservoir-scale. The modelling framework is capable of handling complex geochemical reactions as a function of prescribed flow conditions, water composition and minerals distribution within the rocks. The model is also capable of considering complex porosity feedback based on the relation between flow and chemistry.
In this investigation, we exclusively focus on benchmarking the coupled numerical solver with respect to dissolution and precipitation processes taking place within a single phase system. For the benchmark, we consider well-established datasets available at the pore scale and the continuum scale. This new generation hydro-geochemical modelling platform opens the path to multi-scale reactive transport simulations from the pore- to the reservoir-scale using phase equilibrium and kinetic reactions. The cornerstone of this work is based on the micro-continuum formulation 1, i.e a multi-scale numerical approach that is intermediate between a pure Navier-Stokes description of the transport for which all the porosity is fully resolved and pure continuum-scale modelling based on Darcy's law. This hybrid-scale approach is based on the Darcy-Brinkman-Stokes equation 2 and allows for the three-dimensional modelling of flow and transport in regions free of solids and porous regions in a single framework. The transport is taken care by an open-source CFD toolbox "OpenFOAM"[3] and the chemistry is solved by another open-source geochemical library package "Phreeqc"[4]. The choice for the above mentioned packages is because OpenFOAM and Phreeqc are popular amongst the user community in their respective fields. By considering the coupling proposed across multi-scales and benchmarking the solver, we expect it shall mutually benefit the industrial and academic communities.
Unlike the state-of-the-art hydro-geochemical simulators, our framework not only models processes at the reservoir-scale but it is also well suited to simulate flow, transport, and geochemical reactions in 3D micro-tomography images. We demonstrate the ability of the framework to reproduce microfluidic experiments of reactive systems under single-phase flow conditions. We then consider to extend our work to multiphase systems.

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The Study of Limit Liquid Production Prediction for Porous Medias Deformation Reservoir

Author: Tao CHANG[None]

Co-authors: Jinman LI ; Zhenpeng LI ; Honghui QUAN ; Jianguo LIU

Corresponding Author: changtao@cnooc.com.cn

The prediction of limit liquid production is important to continental deposit oilfield which is in late stage of development. The conventional forecast, based on the Darcy's law to perform linear prediction, which focused on the limit production pressure difference and energy supply level. It assumes that the porous medium, which the fluid flows through, is rigid, the characteristics of the porous medium and the permeability of the reservoir are constant. With shallow burial depth and high crude oil viscosity, unconsolidated sandstone reservoir, which has the characters of high porosity, high permeability, and poor mechanical strength, is widely distributed in the Bohai Bay. High level of liquid production rate was preferred in the late production stage, and good production performance had been received. The characteristics of the reservoir and the way of liquid extraction have caused elastic and plastic changes, deformation of the skeleton and sand production in the porous medium, resulting in the porous media deformation and the fundamental change of the seepage conditions. Without considering these changes, the prediction result is wrong, which has a bad effect on economic and efficient development of offshore oil fields. Based on the experiments of porous sand flow changes, this paper analyzed the factors and laws of deformation of porous media deformation. The change laws were incorporated into the seepage theory, and further deduced Prediction method of liquid production level of Porous Medias Deformation. With this prediction method, the C oilfield in Bohai Bay of China had a fitting effect is only 5%, which is 40% -50% higher than the conventional method.

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Evaluation and comparison of various numerical porosimetry methods: Yield Stress fluids Method, Mercury Intrusion Porosimetry and pore Network Modelling approaches

Authors: Antonio Rodríguez de Castro[1]; Mehrez Agnaou[2]; Azita Ahmadi[3]; Abdelaziz Omari[4]

[1] *Arts et Métiers ParisTech*

[2] *University of Waterloo*

[3] *I2M, Arts et Métiers Paris-Tech, CNRS*

[4] *I2M, Bordeaux-INP, CNRS*

Corresponding Authors: antonio.rodriguezdecastro@ensam.eu, omari@enscbp.fr, magnaou@outlook.com, azita.ahmadi@ensam.eu

Mercury Intrusion Porosimetry (MIP) is still today the reference porosimetry technique despite its environmental health and safety concerns. As a safe alternative, the Yield Stress fluids Method (YSM) consists in computing the Pore Size Distribution (PSD) of a given material from the pressure drop vs. flow rate measurements during injection of a yield stress fluid [1–4]. However, the question arises whether the PSDs provided by YSM are representative of the actual pore dimensions. To answer this question, three numerical methods to obtain the PSD from 2D digital images are proposed and compared in the present work 5. First, direct numerical simulations of YSM tests are performed in the considered media. Then, realistic PSDs are computed from pore Network Models (NM) extracted from the images. Furthermore, the obtained networks are also used to simulate MIP tests. The

quantitative numerical results allow the evaluation of the relevance of YSM as an alternative to toxic MIP. Good agreement is observed between the results obtained with the different approaches. YSM is shown, not only to be an effective experimental alternative to toxic MIP, but also a novel benchmark to analyse images provided by micro-tomography. Moreover, numerical simulations have been confirmed as a powerful tool to investigate the mechanisms affecting micro-scale flow of yield stress fluids in 2D porous media and to illustrate and validate the physical principle of YSM.

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An Embedded Discrete Fracture Method Based Well-Test Model for Pressure Transient Analysis in Fractured Wells with Complex Fracture Networks

Authors: Hui Liu[1]; Xinwei Liao[2]; Xiaoliang Zhao[2]; Lijia Yuan[3]; Juan Zhao[4]

[1] *China University of Petroleum,Beijing*

[2] *China University of Petroleum, Beijing*

[3] *No.2 oil production plant, Changqing Oilfield, China*

[4] *No.2 oil production plant of Changqing Oilfield*

Corresponding Authors: liuhuiguige@gmail.com, 513849056@qq.com, zxl@cup.edu.cn, huiliu012@gmail.com, xinwei@cup.edu.cn

Due to the complexity of shale reservoir geology, hydraulic fractures (HFs), microfractures connected to HFs (MFs) and natural fractures (NFs) can be coupled into an extremely complex fracture network (CFN) around wells after hydraulically fracturing treatments.
Numerous studies have been conducted to investigate the pressure transient responses with fracture networks. However, analytical, semi-analytical or traditional numerical fracture models cannot be applied to the pressure transient analysis of complex and large-scale distributed fractured reservoirs.

Given the imperfections of the existing models, an Embedded Discrete Fracture Method based Well-Test Model (EDFM-WTM) is proposed. The EDFM-WTM shows excellent advantages over the dual-porosity model, dual-permeability model and stripe-fracture model (SFM) in both computational performance and simplicity of simulation workflow due to the use of finite volume method, automatic mesh generation algorithm, automatic differential solving technique, parallel algorithm, and the introduced discrete operators. According to the comparison of calculation results in this paper, the computational performance can be improved by more than 40% compared with that of SFM in the commercial software KAPPA. Finally, based on the EDFM-WTM, we provide a detailed pressure transient analysis of an actual vertically fractured well with different properties of NFs, MFs, and HFs.

The results show that the vertically fractured well with an extremely CFN can be divided into seven flow regimes, including (1) Wellbore storage and skin effect, (2) Bilinear flow , (3) MF-HF supply (”dip 1”), (4) formation linear flow , (5) MF&NF impacts (”dip 2”), (6) pseudo boundary dominated flow, (7) Pseudo radial flow . Sensitivity analysis shows that
(1) The “dip 1” is related to MF-HF supply and the “dip 2” is related to the impacts of MFs and NFs. The properties of MF, such as length, conductivity, intersection angle with HF , have an essential impact on “dip 1” flow regime. The properties of NF, such as the scale, the number, and the conductivity, have an essential impact on the “dip 2” flow regime.
(2) It can be seen clearly from the pressure distribution that both the effective control area of the fracture network and the fluid supply from MF-HF can be maximized if the well is located in the center of the fracture network and the HFs and MFs are perpendicular to each other.

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Coupling Staggered-Grid and vertex-centered Finite Volume Methods for Free Flow/Porous-Medium Flow Problems

Authors: Martin Schneider[1]; Edward Coltman[2]; Kilian Weishaupt[1]; Rainer Helmig[1]

[1] *University of Stuttgart*

[2] *University of Stuttgart IWS-LH2*

Corresponding Authors: kilian.weishaupt@iws.uni-stuttgart.de, martin.schneider@iws.uni-stuttgart.de, edward.coltman@iws.uni-stuttgart.de, rainer.helmig@iws.uni-stuttgart.de

Exchange processes across a porous-medium free-flow interface occur in a wide range of environmental, technical and bio-mechanical systems. In the course of these processes, flow dynamics in the porous domain and in the free-flow domain exhibit strong coupling, often controlled by mechanisms at the common interfaces. Despite every-growing computational capacities, numerical modeling these kind of systems, including the porous geometry, is only feasible for small-scale problems. For larger domain sizes, averaging techniques, involving the concept of a representative elementary volume (REV), are used in order to yield upscaled models for the description of the porous domain. These models can then be coupled to the free-flow region either using a single-domain or a two-domain approach.
In this work, we focus on the two-domain approach, which decomposes the problem into two disjoint subdomains. The free-flow region is then governed by the Navier-Stokes equations while Darcy’s or Forchheimer’s law is used in the porous-medium subdomain 1. Appropriate coupling conditions have to be formulated at the common interface, which enforce the conservation of mass, momentum and energy.

In this work, a new approach (following ideas presented in 2) for the coupling of a staggered-grid finite volume method for the Navier-Stokes equations in the free-flow subdomain and a vertex-centered finite volume method (Box method) to solve Darcy flow in the porous medium is presented.

Using the Box method in the porous domain has the advantage that degrees of freedom are located at the common interface, and therefore allows the interpolation of primary variables (e.g. pressure, temperature or mass fractions) at interfaces. This allows the use of general non-matching grids at the interface and does not require interface solvers, as for example those presented in [3]. Additionally, by using the local bilinear Ansatz functions of the Box method, Forchheimer's law and dispersion concepts can be realized in a straight-forward manner. Furthermore, numerical experiments are presented which demonstrate the applicability of the developed approach for various applications, including compositional, non-isothermal multi-phase flow.

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Reduced-Physics Multilevel Monte Carlo Methods for Uncertainty Quantification in Complex Reservoirs

Authors: Øystein Klemetsdal[1]; Stein Krogstad[1]; Knut-Andreas Lie[1]

[1] *SINTEF Digital*

Corresponding Authors: knut-andreas.lie@sintef.no, stein.krogstad@sintef.no, oystein.klemetsdal@sintef.no

The Monte Carlo (MC) method is an appealing candidate for uncertainty quantification in reservoir simulation for three reasons: (i) It is the preferred approach for systematic reduction in variance for cases with high-dimensional uncertainty with a strongly nonlinear effect (robustness); (ii) it is seamlessly compatible with any reservoir simulator (non-intrusive); and (iii) it is straight-forward to parallelize (embarrassingly parallel). The method does, however, suffer from a painstakingly slow convergence rate of one half. This means that in many cases, an unacceptably large number of samples are required to achieve a sufficiently low variance.

Multilevel Monte Carlo (MLMC) methods were proposed as a work-around for this slow convergence rate. The premise of these methods is that we can approximate the solution at different levels of accuracy, where less accurate approximations are also less expensive to compute. By computing more samples on lower levels, and less samples on higher levels, we can then obtain a low accuracy at a significantly reduced cost compared to a regular MC method. In reservoir simulation, different levels are typically interpreted as different degrees of spatial upscaling. However, complex geomodels (e.g., channelized reservoirs with high-permeability contrast, different rock types and multiphase behavior) may be very challenging to upscale, and the best methods are generally expensive.

Different levels may also be interpreted as different solver accuracy, where a more accurate solver/discretization is used at higher levels - a view taken by a number of authors. In fact, the only requirement for MLMC to work is that the accuracy and cost of computing a sample increases with level, whereas the variance between two consecutive levels decreases with level. Herein, we follow this line of thought, and outline an MLMC method that uses the same fine spatial resolution for all levels. At the finest level, we use a standard fully-implicit finite volume solver, whereas coarser levels use

simple approximate solutions obtained using flow diagnostics and multiscale methods. This gives a flexible and efficient framework for uncertainty quantification that is well suited for geomodels with industry-grade complexity. We demonstrate the applicability of the method on complex geomodels for which efficient upscaling techniques are not readily available, and compare it to standard MC, and MLMC with upscaling.

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The characteristics of gas-phase flow channel under the stratum condition in porous sandstone reservoirs

Authors: Yong Hu[1]; Xizhe Li[1]; Qingyan Mei[2]; Yingli Chen[2]; Xuan Xu[1]; Chunyan Jiao[1]; Qiuying Zhu[1]; Changmin Guo[1]; Chao Qian[1]

[1] *PetroChina Research Institute of Petroleum Exploration & Development, Beijing 100083, China*

[2] *Exploration and Development Research Institute of Petroleum Southwest Oil and Gas Field Company, ChengDu 610041, China*

Corresponding Authors: huy69@petrochina.com.cn, lxz69@petrochina.com.cn

Abstract: The size of the gas seepage channel is one of the key parameters that determines the gas seepage capacity. However, not all pore throats can be effective gas-phase flow channels because of the influence of water saturation and net overburden pressure under stratum conditions. Usually, the difference is significant between the real value and the results tested by experiment in Lab under the conventional condition. So, how to realize it is one of the hard work in lab. Thus, this paper defines the index of gas-phase seepage channel by the ratio of gas permeability under stratum conditions to the conventional ground and simplifies the seepage channel which is composed of complex pore throat in sandstone into a single round tube model based on the principle of flow similarity. So that the paper proposes a mathematical model to evaluate the radius of the gas-phase percolation channel under formation conditions, which achieves the mutual transformation of results between the ground test and the stratum conditions. In this paper, taking the Sulige gas field as the object, the sandstone reservoir with conventional ground permeability which varies from 0.073mD to 25.72mD has been researched. The experiments are carried out under conditions that net overburden pressure is 40.8MPa and the water saturation (Sw) are 0%, 30%, 40%, and 50% respectively. The results indicate that there are significant differences in the effects of water saturation on sandstone reservoirs with different permeability. For tight sandstone with permeability(K) less than 0.1mD, the main gas-phase flow channel radius under stratum conditions(Sw=30, 40, 50%) is less than 0.1μm, which is decreased by 60.0% to 93.0% compared to the ground conditions(Sw=0%); For sandstone reservoirs with K between 0.1 and 1.0mD, the main gas-phase flow channel radius under stratum conditions(Sw=30, 40, 50%) is less than 0.5μm, which is decreased by 20% to 75% compared to the ground conditions(Sw=0%); For sandstone reservoirs with K more than 1.0mD, the main gas-phase flow channel radius under stratum conditions(Sw=30, 40, 50%) is bigger than 0.3μm, which is decreased by less than 40% compared to the ground conditions(Sw=0%). It is of great theoretical and practical significance for the effective development of those kind of gas reservoirs.
Key words: porous sandstone reservoirs; gas-phase flow channel; under the stratum condition sandstone; experiment study; mathematical model

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A Bundle of Capillary Tubes (BOCT) Model for Carbonated Water Flooding (CWF); a Promising Technique for Simultaneous CO2 Storage and Enhanced Oil Recovery Purposes

Authors: Puyan Bakhshi[1]; M. Mercedes Maroto-Valer[2]; Mohammad Amani[1]

[1] *Heriot-Watt University*

[2] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, UK*

Corresponding Authors: pb62@hw.ac.uk, ma399@hw.ac.uk, m.maroto-valer@hw.ac.uk

Carbonated water flooding (CWF) is a promising technique for EOR and a suitable methodology for permanent geological sequestration of CO2. As carbonated water contacts oil, CO2 preferably diffuses from water into oil, resulting in oil displacement mainly due to oil swelling and viscosity reduction. Moreover, as CO2 remains dissolved in the fluids rather than staying as a free phase, the risk of buoyancy-driven leakage is minimised.

To date, extensive experimental studies have been performed on the EOR and CO2 storage potential of CWF. Nonetheless, due to the complexity of this process, numerical studies on accurate modelling of CWF are limited. Using commercial and in-house simulators, a number of studies have been conducted which exhibit promising results in investigating the underlying mechanisms of this process and predicting experimental observations [1-3]. However, scarcity of experimental data for predicting important parameters and model validation, as well as the intrinsic complexity of the CWF process, cause severe challenges for conducting numerical studies. Accordingly, the deficiencies of previous models, such as over-prediction of oil recovery, unrealistic conditions or materials, over-complex numerical codes, etc. necessitate new avenues of investigation.

Here, we present a convenient, versatile numerical model capable of capturing the complex nature of CWF's EOR mechanisms with relatively low runtimes. We developed a bundle of capillary tubes (BOCT) model to numerically simulate the results of a previously published experimental study on CWF in core samples [4].

In this numerical study, a pseudo-compositional approach is applied. Firstly, a BOCT model is employed to be a representative of the porous media. Subsequently, the fluid flow equations were derived using momentum balance. Then, through the utilization of a lumped mass transfer approach, CO2 distribution through the media is captured by considering two phases (water and oil) and three components (water, oil, and CO2). Finally, the contribution of CO2 in the EOR process is modelled by using the calculated CO2 distribution throughout the medium and employing valid, widely used correlations.

It was shown that the developed model is adequately capable of matching the oil recovery levels outlined by the experimental results. In addition, sensitivity analyses were performed to investigate the influence of different parameters on oil recovery by CWF and validate the main underlying EOR mechanisms, specifically oil swelling and viscosity reduction. These analyses confirmed oil viscosity and API as the main parameters affecting the performance of the EOR process. Therefore, the BOCT model can be considered as a 'physical experiment'and the assessed performance (pressures, flow rates, and production rates) of such 'samples'of the porous media as 'experimental results'. Finally, by using this model to predict the performance of the CWF process, implementing further costly and time-consuming experimental studies to attain direct measurements can be avoided.

Acknowledgement

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (MILEPOST, Grant agreement no.: 695070). This paper reflects only the authors'view and ERC is not responsible for any use that may be made of the information it contains.

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Extended finite element analysis of a coupled fracture-reservoir model

Author: Elisa Bergkamp[1]

Co-authors: Clemens Verhoosel [1]; Joris Remmers [1]; David Smeulders [1]

[1] *Eindhoven University of Technology*

Corresponding Authors: e.a.bergkamp@tue.nl, d.m.j.smeulders@tue.nl, j.j.c.remmers@tue.nl, c.v.verhoosel@tue.nl

Understanding the interaction between a fracture flow and a deformable porous medium is essential for geomechanical applications such as Enhanced Geothermal Systems, the controlled extraction of oil and gas from fractured reservoirs, and CO2 sequestration. To study this interaction we developed a coupled fracture-reservoir model. In the model, the fracture flow is described by the Stokes equations, the porous formation is described by Biot's equations, and the fluid flow in the formation is described by Darcy's law. Both the fracture flow region and the formation are saturated with fluid.

One of the challenges addressed in this contribution is the choice and implementation of suitable coupling conditions on the shared interface of the fracture flow and the poroelastic medium. To fully couple the Stokes equations to Biot's equations, both stress and flow conditions are prescribed. The slip encountered by the fluid flowing along the saturated formation is enforced by the Beavers-Joseph-Saffman condition [1,2]. Furthermore, the Darcy flux over the interface is driven by a pressure jump condition, as introduced by Showalter [3].

In the subsurface setting, fractures generally have an aperture which is much smaller than their length. As such, resolving the length scale associated with the aperture of the fracture is computationally impractical. Therefore, we represent the fractures as lower-dimensional geometries, on which we solve a dimensionally-reduced flow model. Representing the fractures as lower-dimensional geometries enables us to extend the model to include fracture propagation. The lower-dimensional representation also enables the use of standard fracture propagation models.

We solve the coupled fracture-reservoir problem using a staggered FEA approach. The fracture is described using the XFEM framework [4], using a local enrichment of the pressure in the fracture to mimic the pressure jump condition [3]. Results of the coupled model are validated using analytical results and literature benchmarks.

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Data-driven models based on flow diagnostic and machine learning techniques

Authors: Manuel Borregales[1]; Stein Krogstad[1]; Knut-Andreas Lie[1]

[1] *SINTEF Digital*

Corresponding Authors: stein.krogstad@sintef.no, knut-andreas.lie@sintef.no, manuel.borregales@sintef.no

Data-driven models for waterflooding are an attractive alternative for forecasting and schedule optimization when a full-scale reservoir simulation model is computationally prohibitive [3, 4]. A calibration process of the data-driven model is necessary for a satisfactory forecast. However, a lot of data is needed to forecast the flow distribution between the injectors and producers accurately. Mature fields come with enough data to calibrate the model, but younger fields and new developments require a different approach to compensate for the lack of historical data. Here, we use flow diagnostic to obtain, from an existing reservoir simulation, the volumetric information about reservoir portioning and inter-well communication between injectors and producers.

Flow diagnostics refers to a set of simple and controlled numerical flow experiments that are run to probe a reservoir model, establish connections and basic volume estimates, and quickly provide a qualitative picture of the flow patterns in the reservoir 1. We used the flow diagnostics module in MRST 2 to rapidly set up a data-driven model composed of a network of 1D inter-well connections. The calibration process of the model is simple
and computationally inexpensive.

The saturation front on each 1D inter-well connection is obtained numerically by finite-difference methods and machine learning techniques. Several numerical examples will be presented, pointing out the advantages and limitations of this new methodology. This approach is robust for complex reservoirs with multiphase flow.

Keywords—data-driven model, history matching, waterflooding, machine learning, optimal scheduling

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Investigation of salt-precipitation processes in porous-media systems at the pore scale

Author: Theresa Kurz[1]

Co-authors: Rainer Helmig [1]; Douglas Meisenheimer [2]; Dorthe Wildenschild [2]

[1] *University of Stuttgart*

[2] *Oregon State University*

Corresponding Authors: dorthe@engr.orst.edu, theresa.kurz@iws.uni-stuttgart.de, meisenhd@oregonstate.edu, rainer.helmig@iws.uni-stuttgart.de

The fundamental understanding of salt precipitation in porous media due to evaporation processes is important in different environmental and technical applications. For example salt precipitation in building materials generates stresses, which can lead to weathering and damage of constructions and cultural monuments. The salinization of soil in arid and semi-arid zones and the resulting reduction of crop yield is a further challenge.
During the evaporation of a salt solution, the salt concentration increases at the evaporation front and solid precipitates in the porous media when the solubility limit is exceeded. Here, many process controlling properties operate on the pore scale, such as the spatially varying salt concentration and the modification of pore space due to pore clogging.
To investigate these pore-scale processes, experiments were conducted at the microCT imaging facility at Oregon State University. A column filled with glass beads and potassium-iodide solution was scanned after several periods of evaporation at the column top using X-ray micro-tomography. From those images, the distribution of the brine and air phases as well as the location of precipitated solid salt, can be determined and analysed.
Further, the processes are modelled using a pore-network model, implemented in DuMu^x, an open-source, porous-media flow and transport simulator. A pore-network model efficiently resolves pore-scale phenomena using a network of one-dimensional entities. Therefore, reactive transport including an equilibrium reaction for the precipitation of salt and the resulting change in pore-space volume is implemented.
With the comparison of the detailed experiment and simulation results, fundamental understanding of the processes at the pore scale during salt precipitation in porous media will be gained, and relevant processes will be determined.

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Mathematical analysis of foam flow in porous media

Authors: Grigori Chapiro[1]; Luis Fernando Lozano[1]; Rosmery Zavala[1]; Pacelli Zitha[2]

[1] *Universidade Federal de Juiz de Fora*

[2] *TU Delft*

Corresponding Authors: rosmery.quispe@hotmail.com, grigorichapiro@gmail.com, luisfer99@gmail.com, p.l.j.zitha@tudelft.nl

Foam is a dispersion of gas in a continuous liquid stabilized by surfactants. Its behavior in porous media gives rise to a number of interesting features having applications in geological energy and storage, enhanced oil and gas recovery as well as materials science and engineering. With some additional assumptions, one-dimensional foam displacement can be represented by a system of partial differential equations. Using the fractional-flow methods, an application of the method of characteristics, we solve the corresponding Riemann problem for this model. The methodology combines theoretical analysis with numerical experiments to provide scientific evidence for the existence (and

stability) of solutions. Some mathematical properties of the model will be presented supported by direct numerical simulations.

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Implicit multiscale modelling for stress-dependent permeability in a poroelastic dual-continuum setting

Author: Mark Ashworth[None]

Co-authors: Florian Doster ; Christine Maier [1]

[1] *Heriot-Watt University*

Corresponding Authors: c.maier@hw.ac.uk, f.doster@hw.ac.uk, ma174@hw.ac.uk

Deformation of fractured porous media is well known to affect material properties such as permeability. The focus of this work is to incorporate stress-dependent effective fracture permeability into a poroelastically coupled dual-continuum (DC) framework. In this modelling concept the continua are defined as homogenised equivalents of fine-scale poroelastic constituents. In order to generate the homogenised stress-effective permeability data used at the DC scale, we employ an implicit multiscale modelling approach. For this approach a suite of fine-scale explicit simulations is run prior to (macroscopic) DC simulation. In the ensemble of fine-scale simulations we vary stress components and pressures for given constituent material geometries. The resulting discrete data is then augmented by way of a non-linear interpolator for usage in the automatic differentiation framework of the Matlab Reservoir Simulation Toolbox (MRST). In the current work, we consider permeability evolutions at the fine-scale simply through an aperture coupled parallel plate model. However, extensions to concepts incorporating surface roughness at the fine-scale, for example, are straight forward. The implicit multiscale modelling approach thus allows us to change local stress-permeability relations without ever having to write explicit macroscopic stress-effective permeability relations. One can therefore incorporate the fidelity of fine-scale explicit models with the practicality of homogenised multi-continuum models. To test the framework, we apply it to the modelling of a prototypical 2D poroelastic problem, as well as a subsurface depletion problem.

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Studying the effects of heterogeneity on karstification and wormholing phenomena using Operator Based Linearization and High-Resolution LiDAR data

Author: Stephan de Hoop[1]

Co-authors: Denis Voskov [1]; Giovanni Bertotti [1]

[1] *Delft University of Technology*

Corresponding Authors: s.dehoop-1@tudelft.nl, d.v.voskov@tudelft.nl

Rising demand for cleaner energy sources, e.g. geothermal energy, has led to the extensive investigation of high-enthalpy carbonate reservoirs. These reservoirs are often chemically and mechanically altered and hence contain a large uncertainty in the spatial distribution of the reservoir parameters. The resulting discontinuity features commonly include complex fracture networks, large interconnected cave systems, and other various flow barriers/conduits. Several conceptual/qualitative models exists, however, it is not fully understood what are the main driving forces behind the resulting geometry of the networks and if quantitative predictions can be made based on these models. This further complicates the reservoir modelling process, both the static reservoir characterization and the dynamic response for uncertainty analysis. In order to improve the reservoir characterization, high-resolution LiDAR datasets from several outcrops were acquired, i.e. caves that were accessible with a portable LiDAR scanner. A statistical analysis is performed on the geometry of the resulting cave networks. Linking the processes of wormholes creation, with the aid of numerical simulations, and the measured manifestation of the discontinuity networks will substantially improve the reservoir modelling process and subsequent uncertainty quantification workflow.

Furthermore, in order to successfully develop these cleaner energy resources and have an effective management of the associated risks, it is required to evaluate the large ensemble of multiphase reactive flow and transport simulations. This has led to the development of an efficient element based reduction technique which can significantly decrease the number of conservation equations and thereby reduce the computational time. In this approach, components or chemical species are translated to their constituent elements using chemical and thermodynamic equilibrium relations. Next, a finite-volume unstructured discretization in space is applied together with a fully-implicit approximation in time. The resulting complex nonlinear system is parameterized using the Operator Based Linearization (OBL).

The OBL framework transfers the governing nonlinear Partial Differential Equations into a linearized operator-form where the Jacobian is constructed as a product of a matrix of derivatives with respect to state variables and discretization operators. The state-dependent operators are only evaluated adaptively at vertices of the mesh introduced in the parameter-space. The continuous representation of state-dependent operators as well as their derivatives is achieved by using a multi-linear interpolation in parameter-space. This means that the usually time-consuming phase and chemical equilibrium computations, performed on each nonlinear iteration and in every control volume, are only executed when evaluating the operators in the new supporting points, thereby significantly reducing both the linearization time and the number of nonlinear iterations. Recently the reactive transport module was extended to include both kinetic reactions and the coupling with PHREEQC which allows to include more complex chemical interactions.

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Modelling of long-term along-fault flow of CO2 from a natural reservoir

Authors: Jeroen Snippe[1]; Niko Kampman[1]; Kevin Bisdom[1]; Tim Tambach[1]; Rafael March[2]; Tomos Phillips[2]; Nathaniel Forbes Inskip[3]; Florian Doster[4]; Andreas Busch[2]

[1] *Shell Global Solutions International B. V.*

[2] *Heriot-Watt University*

[3] *Heriot-Watt*

[4] *Heriot Watt University*

Corresponding Authors: niko.kampman@shell.com, a.busch@hw.ac.uk, n.forbes_inskip@hw.ac.uk, jeroen.snippe@shell.com, tp45@hw.ac.uk, r.march@hw.ac.uk, f.doster@hw.ac.uk, kevin.bisdom@shell.com

Geological sequestration of CO2 requires knowledge of the flow properties of fault-related fracture networks in the low-permeability shale caprocks that overly most of the considered storage sites. A safe, sustainable and economical storage operation requires a profound understanding of these risks, recognising that quantification is challenging due to the many length and time scales involved and the very limited availability of data. The Green River site in Utah is a rare case of leakage from a natural CO2 reservoir, where CO2 (dissolved or gaseous) migrates along two fault zones to the surface. This provides a unique opportunity to understand CO2 leakage mechanisms and volumes along faults. A successful modelling of measured leakage rates will provide confidence in modelling approaches and will help select safe storage sites, de-risk storage operations and guide containment monitoring.
Here, we present an integrated workflow to model the measured leakage rates and locations at this site. We combine laboratory experiments to obtain single-fracture stress-sensitive permeabilities; single-fracture modelling for stress-sensitive relative permeabilities and capillary pressures; fracture network characterisation and modelling for the primary and secondary caprocks; upscaling of properties and constitutive functions in fracture networks; and full compositional flow modelling at field scale modelling. Our results predict locations accurately and, within an order of magnitude, leakage rates correctly without extensive history matching. Subsequent history matching achieves accurate leak rate matches within a-priori uncertainty ranges for model input parameters.

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Research collaboration Highlights: A tribute to Rainer Helmig

Author: Al Cunningham[1]

[1] *Center for Biofilm Engineering, Montana State University*

Corresponding Author: al_c@montana.edu

The Center for Biofilm Engineering (CBE) at Montana State University (MSU) has enjoyed a long-term research collaboration with Professor Rainer Helmig and colleagues at the University of Stuttgart. This collaboration has focused on the evolution of a novel technology for permeability modification in porous media and fractures using a process known as Microbially Induced Calcite Precipitation (MICP). The CBE has focused on MICP experimental research and development at various scales of observation while Stuttgart researchers have developed simulation models which guided experimental work and, ultimately, facilitated successful field testing of MICP for sealing wellbore leakage. Highlights of this decade-long collaboration will be presented with the intention of providing an "entertaining scientific"summary of our productive, enjoyable, and sometimes humorous collaboration with Rainer and colleagues.

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Equivalent Permeability Prediction of Karst Core Samples Using Deep Learning

Authors: Monique Dali[None]; Sergio Ribeiro[1]; Frederico Gomes[1]; Marcio Carvalho[1]

[1] *Pontifícia Universidade Católica do Rio de Janeiro*

Corresponding Authors: fcgomes@lmmp.mec.puc-rio.br, msc@lmmp.mec.puc-rio.br, sergio@lmmp.mec.puc-rio.br, mfeitosa@lmmp.mec.puc-rio.br

Karst carbonate rocks are characterized by the presence of complex structures composed by free flow domains such as fractures, vugs, large pores and cavities 1. High heterogeneity of carbonates makes the prediction of permeability a challenge. The presence of vugs has a substantial effect on the flow characteristics and favors the formation of flow preferential paths.

Micro-tomographic images of coquinas core samples were obtained and segmented into two regions (one containing vugs and one containing the porous matrix). Canny 2 edge detection technique was used to digitize the segmented images and the two regions were divided using triangular finite element meshes. The two-dimensional flow through the porous matrix and vugs was solved [3] using the Brinkman [4] formulation with a penalization term 5. The equivalent permeability of each sample was determined based on the flow predictions.

Despite the advances in robust solvers and parallel computing, running numerical simulations for larger domains is still not practical. Metaheuristics and data-based models have been used to mimic complex physical processes and reduce considerably inference calculation time [6].

The present work focuses on investigating the use of neural networks with convolutional layers (CNN) to recognize vug patterns in binary images of carbonates and how it correlates with the equivalent permeability. Convolutional Neural Networks have proven to be suited for image pattern recognition [7] when trained with a large number of images. Therefore, around six thousand images from 2D slices of coquinas core samples were used as a training and validation set to CNN.

Different from usual classification schemes found in literature, this research applies a supervised approach using simulated equivalent permeability as prediction target related to each macropore structure pattern.

Results presented an average prediction accuracy of 94% in the test set (unseen patters of vugs and caves), even with macroporosity values above 20%. Further tests will be performed to evaluate the prediction capabilities at even higher macroporosity values and different rock formation types.

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The impact of fracture surface roughness on stress dependent permeability

Authors: Amanzhol Kubeyev[1]; Christine Maier[2]; Niko Kampman[3]; Kevin Bisdom[3]; Rafael March Castaneda Neto[2]; Florian Doster[2]

[1] *HERIOT-WATT*

[2] *Heriot-Watt*

[3] *Shell*

Corresponding Authors: f.doster@hw.ac.uk, ak87@hw.ac.uk, c.maier@hw.ac.uk, niko.kampman@shell.com, r.march@hw.ac.uk, kevin.bisdom@shell.com

The magnitude of flow through fractures is a large uncertainty in subsurface flow modelling. The conductivity of fractures is extremely sensitive to the aperture, which in turn, depends on stress conditions.Stress dependent permeabilities of fractured reservoir rocks can be measured in the laboratory on core scale. However, a systematic understanding of the behaviour of stress sensitive fracture apertures on field scale and the primary parameters that determine that behaviour is still lacking. Furthermore, the predominantly used correlations of effective stress on fractures and their aperture were developed for low confinement pressures such that they might not be applicable for reservoir rocks under subsurface conditions.

Here, we aim to improve the understanding of the contribution of fracture roughness to the stress-permeability relationship. We present systematic numerical investigations using an inhouse developed solver for quasi-static discrete interacting elastic continua that includes contact detection and contact interaction algorithms using Lagrange multipliers in 2D cross sections. This code allows us to study the opening and closing of fractures. It is based on the geomechanics solver of the Matlab Reservoir Simulation Toolbox (MRST) on the Virtual Elements Method (VEM) augmented by contact detection and contact interaction algorithms using Lagrange multipliers in 2D cross sections. We solve Stokes equations to obtain the permeability under different stress conditions perpendicular to the plane. We assess the different methodologies to measure roughness and their correlation with the stress-permeability relationship while using fracture surface profiles that are obtained from rock samples and synthetically generated ones. We also investigate the impact of several offsets of surfaces mimicking the effect of shear induced dilation of the fracture apertures.

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Applications of the electromagnetic heating in EOR

Author: Samuel Almeida[None]

Co-authors: Grigori Chapiro [1]; Pacelli Zitha [2]

[1] *Universidade Federal de Juiz de Fora*

[2] *TU Delft*

Corresponding Authors: grigorichapiro@gmail.com, p.l.j.zitha@tudelft.nl, samuelufjf@gmail.com

One potential technique used to explore heavy and medium viscosity oil fields consists in water injection, which is heated by high frequency electromagnetic waves resulting in the viscosity decrease and consequent increase in the mobility. We propose two-dimensional mathematical model based on partial differential equations describing the energy balance and the water mass conservation.

These equations are solved analytically for a simplified case, which is used to validate the numerical implementation. The analytical solution is based on the Fourier's method. It was done for the two-dimensional case in the rectangular domain and also in the cylindrical domain with radial symmetry. Numerical results show how the electromagnetic heating impacts the oil recovery factor in the five spot geometry.

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3D Visualization of Oil Displacement by a Suspension of Microcapsules

Author: Raphael Chalhub Oliveira Spinelli Ribeiro[1]

Co-author: Marcio Carvalho [2]

[1] *PUC-Rio*

[2] *Pontifícia Universidade Católica do Rio de Janeiro*

Corresponding Authors: msc@lmmp.mec.puc-rio.br, raphael@lmmp.mec.puc-rio.br

In this work, we used confocal laser-scanning microscopy to study the fundamentals of oil displacement in porous media, which enables a 3D reconstruction of the pore space and visualization of the evolution of phase saturation during the process.

We explored the effect of injecting an aqueous suspension of flexible microcapsules on oil displacement. During the setup and fluids preparation, each phase (including the inner phase of the microcapsules) was mixed with a different fluorescent pigment, which enabled the visualization of the three phases (oil, water and capsules) simultaneously. The microcapsules were produced using a non-planar microfluidic device which enabled to precisely control their size and shell thickness.

The transparent porous devices comprised of sintered packing of glass beads. In some of the experiments, we used beads of different diameters to form a stratified porous media, with layers with different permeabilities. The porous media were initially fully saturated with oil. First, oil was displaced by the injection of water until no oil has been produced. Water injection was followed by the injection of the microcapsule suspension.

Image processing was used to quantify the volume of trapped oil after water and microcapsule suspension injection. The microcapsules were able to divert the water phase and mobilize trapped oil ganglia, showing great potential to be used as an enhanced oil recovery method. The simultaneous visualization of the three phases combined with image analysis enabled fundamental understanding of the pore scale phenomena associated with oil displacement by water and soft microcapsule suspension.

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Evaluation of Equivalent Permeability in 3D Vuggy Porous Media using Brinkman Model and Digital Image Analysis

Author: Rafael Cruz[1]

Co-authors: Marcio Carvalho [1]; Frederico Carvalho [1]

[1] *Pontifical Catholic University of Rio de Janeiro*

Corresponding Authors: rmoura@lmmp.mec.puc-rio.br, msc@lmmp.mec.puc-rio.br

Macroscopic rock properties such as porosity, permeability, and wave velocity describe petrophysical characteristics of rocks. In the particular case of carbonates, the estimation of equivalent petrophysical properties is challenging because of the presence of distinct rock structures in the same domain of interest 1. Also, the presence of voids with sizes of disparate order of magnitude imposes extra difficulty to predict equivalent properties in carbonates. Equivalent properties can be determined through experimental measurements in laboratory, which can be relatively slow and expensive, or via numerical simulation. In this study, we determined equivalent permeability of vuggy porous media using a Digital Rock Physics workflow [2, 3], which comprised of microCT scan of the rock sample, mesh generation [4] on the porous matrix and vuggy regions and the solution of the Brinkman model 5 using the finite element method [6]. Digital Image Analysis (DIA) was used to determine the characteristics of the macro pores (volume, surface area, pattern, among others), which were use to curve-fit the solutions of the Brinkman model and the calculation of the equivalent permeability of different samples. The goal was to be able to evaluate the equivalent permeability simply based on the image characteristics of the sample, without the need of solving the Brinkman model.

Due to the scale problem related to the presence of voids (cavities, large fractures) in various sizes, the physical model proposed by Brinkman was chosen to describe the flow through the rock sample. Brinkman proposed an average model in which the regions with micropores are considered to be a porous media obeying the Darcy law, while the flow through voids is described by Stoke's law. The equivalent permeability was obtained by numerically emulating Darcys experiment between the inlet and outlet boundaries. For the DIA, the considered parameters for generating the empirical function were the rock's macroporosity, the surface area of the voids, the standard deviation of the voids' centroids, and a proposed parameter that considers the dispersion of the structure of each disconnected void. In order to generate sufficient data for the digital computational analysis, several 3D cuboid fragments were extracted from two digital coquina rock samples and the results of each of them were compared in order to recognize if the results were sample dependent. Also, the dimension of the cuboid domain was determined by defining a representative elementary volume through the investigation of the rock's macroporosity on different scales. Preliminary results show for one coquina sample that the proposed model is able to predict the equivalent permeability of the rock with almost 90\% of certainty according to the R-square statistical measure. These results show not only a powerful equation for evaluating the equivalent permeability of rock samples but also reveals insights on the core parameters, besides the macroporosity, that influence rock properties.

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Polymer Screening Using Microfluidics

Author: Mohammad Zargartalebi[1]

Co-author: Anne Benneker [1]

[1] *University of Calgary*

Corresponding Authors: anne.benneker@ucalgary.ca, mohammad.zargartaleb@ucalgary.ca

The world's energy demand is increasing every year and hydrocarbon resources still make up more than 55% of the energy consumption. As such, several enhanced oil recovery (EOR) methods are applied to improve hydrocarbon production from conventional and unconventional sources. Among various EOR methods, polymer flooding is a promising method, which has been applied since the late 1960s. In this method, the high viscosity of the polymer solution results in an increased reservoir sweep efficiency. Despite wide application of polymer flooding, polymer retention is still a limiting factor in its performance. Therefore, the most important factor determining successful polymer injection is the ability to predict polymer retention in porous media prior to the field application. This experimental study aims at providing a clear understanding of polymer retention mechanisms using microfluidics. We screen different sizes of polymers through various sizes of microchannels, mimicking different pore sizes and tortuosity found in reservoirs, to determine the main entrapment mechanism. Pressure drop analyses along with fluorescent microscopy aids the explanation of the trapping mechanism by using hydrodynamic behavior of the system and polymer tracking in porous medium. Rheological studies disclose the polymer rheological properties before and after injection. Results show that even when the polymers survive passing through the microchannels, their rheological properties do not persist, changing their efficiency and behavior in polymer flooding processes.

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Absolute Adsorption of Methane in Kerogen Nanoporous Media: Simulation, Characterization and Modeling

Authors: Wanying Pang[1]; Zhehui Jin[1]

[1] *University of Alberta*

Corresponding Authors: wanying@ualberta.ca, zhehui2@ualberta.ca

Accurate estimation of methane adsorption amount is essential for reliable gas-in-place (GIP) evaluation as well as well productivity. While only excess adsorption isotherm is directly measured in experiments, absolute adsorption which represents the actual adsorption amount should be converted from the excess adsorption. However, questions often arise regarding the applicability and accuracy of different conversion methods. In previous molecular simulation works, it has been revealed that methane adsorbed phase density depends on pressure and temperature, indicating that the constant predetermined adsorbed phase density may become inapplicable for absolute adsorption description. Moreover, the widespread pore size distribution (PSD) in shale media leads to different adsorption mechanism in micropores and mesopores. Recent emphases of our studies have been placed on the necessity of explicitly considering PSD in shale and systematic assessment of different conversion method. We found that Ono-Kondo (OK) model can be potentially applied to account for not only pore filling in micropores but also transition zone effect in mesopores. However, the previous model only contains some typical nanopore sizes and the corresponding adsorption types as characterized by grand canonical Monte Carlo (GCMC) simulation and the tested pore sizes are below 10 nm. In this work, following our previous studies, the methane adsorption behavior in various sizes of nanopores is investigated via molecular simulation. The methane adsorption in nanopores is divided into seven adsorption types based on density profiles from GCMC simulation and the characterized adsorption models with lumping method in terms of corresponding pore size are applied in the OK model. The validity of our proposed OK model is examined by 1000 sets of artificially generated PSDs with finely defined pore sizes from 0.7 nm to 30 nm. We find that by fitting the excess adsorption isotherm, OK model coupled with new adsorption models has an excellent agreement in terms of absolute adsorption amount with that obtained from GCMC simulation associated with PSD effect. Our work shows the applicability of OK model for the accurate calculation of methane absolute adsorption in kerogen nanoporous media and should provide important insights into evaluation of gas-in-place in shale reservoir.

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Gravity Segregation in Foam Mobility Control in Heterogeneous Reservoir

Authors: Xiaocong Lyu[1]; Denis Voskov[2]; William Rossen[1]

[1] *Delft University of Technology*

[2] *TU Delft*

Corresponding Authors: w.r.rossen@tudelft.nl, d.v.voskov@tudelft.nl, x.lyu@tudelft.nl

Foam propagation in heterogeneous porous media, especially with gravity segregation, is still a big challenge for conventional foam simulation due to the strongly nonlinear physics. To assess foam transport for enhanced oil recovery (EOR) processes, an accurate prediction of foam behaviour in porous media is essential. In this study, we examine the effects of permeability and gravity segregation on foam propagation. For nonlinear analysis, we use an extension of an Operator-Based Linearization (OBL) approach proposed recently1.

Foam in porous media is often described using an implicit-texture (IT) model with two flow regimes. The OBL approach is applied to reduce the nonlinearity of the foam problem by transforming the discretized conservation equations into space-dependent and state-dependent operators. In this work, we first validate the numerical accuracy of the foam simulation with OBL by comparing a 1D foam simulation using the IT foam model with Newtonian rheology to the fractional-flow solution. Next, the foam-model parameters for four sandstone formations ranging in permeability from 6 to 1900 mD are used to represent a hypothetical reservoir containing four communicating layers2. We compare simulations of gravity segregation in these 2D heterogeneous layered reservoirs with permeability increasing, decreasing, varying randomly from top to bottom layer respectively. We then investigate the effect of reservoir inclination on foam flow with gravity segregation by comparing up-dip versus down-dip co-injection. Finally, we apply our approach to realistic reservoir models with heterogeneity.

The numerical results of the 1D foam model show good agreement with analytical solutions. Permeability affects both the mobility reduction of wet foam in the low-quality-foam regime and the limiting capillary pressure at which foam collapses. Simulation results demonstrate that with a more severe heterogeneity, segregation length can differ significantly, especially for a tilted reservoir.

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Using 2D seismic line data to estimate the possible impact of large-scale and sub-scale structural trapping in the Gassum Formation on the Norwegian Continental Shelf

Author: Odd Andersen[1]

Co-authors: Anja Sundal [2]; Halvor Nilsen [1]

[1] *SINTEF Digital*

[2] *Dept. of Geosciences, University of Oslo*

Corresponding Authors: anja.sundal@geo.uio.no, odd.andersen@sintef.no, halvormoll.nilsen@sintef.no

When storing CO2 in (semi)open, sloping aquifers, the injected CO2 is expected to migrate upslope over time. The realizable storage potential for formations without closed lateral boundaries thus depends on the combined effects of physical and chemical trapping mechanisms in limiting long-time migration out of the designated storage zone. One important such mechanism is the topography of the caprock surface, where parts of the migrating CO2 plume may become trapped in large or small structural pockets along the migration path. Even when such traps are too small to be accurately described by seismic data, they still hold the potential to retard plume migration and trap CO2. This has been explored by several past studies.

In this study, we aim to use real (but scarce) data to estimate the potential of caprock topography to retain migrating CO2 and slow down plume advancement, using the Gassum Formation on the Norwegian Continental shelf as a case study. The top surface of this formation is gently sloping, and characterized by a number of macro-scale structural traps, a few large faults, a large number of small faults, and small-scale depth variations that can be inferred and extrapolated from the seismic data. We seek to estimate the amount of macro- and sub-scale trapping potential of the formation based on a few dozen interpreted 2D seismic lines and identified faults. The seismic lines pass through the are of study at various angles. A number of medium and large faults could be explicitly identified and mapped, as they correlate between several of these lines. In addition, hundreds of small-scale faults are only visible as discontinuities along individual lines. The extent and shape of these small faults between the seismic sections cannot be explicitly known from the data.

In order to investigate structural trapping potential, we generate multiple possible high-resolution realizations of the top surface, constructed to be faithful to both large-scale topography and small-scale statistical properties. Small-scale irregularities are modeled using estimated variograms to

generate Gaussian random fields, while the number and size distribution of minor faults is obtained from statistical analysis along with synthetic fault models.

The structural trapping and plume retardation potential of these top surfaces is subsequently estimated using spill-point (static) analysis and dynamical flow simulation. By applying these techniques on a large ensemble of top surface realizations generated using a combination of stochastic realizations and systematic variation of key model parameters, we seek to explore the range of possible impacts on plume advancement, trapping and migration direction.

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Physics-informed machine learning of permeability prediction and upscaling of reactive transport in porous media

Author: Hongkyu Yoon[1]

[1] *Sandia National Laboratories*

Corresponding Author: hyoon@sandia.gov

Reactive transport in porous media is fundamental to understanding coupled processes for various subsurface energy activities and environmental applications such as geologic carbon storage, subsurface energy recovery, and environmental fate and transport. Over the past few years machine learning methods have been used for image processing, wave data analysis, and classification problems. One of main challenges in conventional machine learning/deep learning for scientific and engineering domains is how we can incorporate physics-informed constraints into training process. The physics-informed or scientific machine learning can provide a new means to improve model prediction by overcoming overfitting to training data so that the trained model can be applicable for more general conditions. In this work we improved the prediction of permeability in porous media using convolutional neural network (CNN) with physics-informed quantities of pore topology characteristics (e.g., porosity, surface area, connectivity) during training stage. Key architectural aspects of machine learning methods will be presented to improve the model predictability. Second, high fidelity pore scale simulations in various pore structures are performed to generate the outcome of reaction transport processes including precipitation and dissolution. The simulation outcomes will be used to develop a reduced order model to reflect the response surfaces under various environmental conditions. In particular, the change of true reactive surface area during reactive transport will be incorporated into a machine learning training process since this reactive area can be significantly different from geometric based reactive area. Comparison of pore-scale reactive transport and physics-informed ML approaches will be presented to discuss an upscaling strategy of reactive transport problems.
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Experimental study on enhanced oil recovery of offshore heavy oil reservoirs by activated water flooding

Author: Xin Chen[1]

Co-authors: Yiqiang Li [1]; MingYue Sui [1]; Jian Zhang [2]; Han Zhang [1]

[1] *China University of Petroleum in Beijing*

[2] *CNOOC Research Institute Beijing*

Corresponding Authors: suimingyue@163.com, cz_cup0709@163.com, zhangjian@cnooc.com, 89731007@163.com, zhanghan@163.com

The bohai oil region in China is a typical offshore heavy oil reservoir with low water drive recovery and further enhanced recovery replacement technology is needed. Hot water flooding is widely used in the development of offshore heavy oil reservoirs, but its effect is restricted by heat loss and relatively low enthalpy. The activated water of heavy oil can make up for the poor viscosity reduction effect of hot water at low temperature and has a synergistic effect with hot water to greatly improve the recovery of heavy oil reservoirs. The activated water of heavy oil is a low molecular weight amphiphilic polymer solution formed by the copolymerization of several functional monomers, and it can enhance viscous oil viscosity reduction effect by emulsifying and dispersing. In this paper, the optimal activated water system was selected by evaluating the viscosity reducing, interfacial activity, and emulsifying performance. The influence of injection speed and oil-water ratio on emulsifying property of the system was analyzed by co-injection experiment. The synergistic effect of activated hot water was obtained by long core displacement experiment. The results show that the activated water DN-1 has the best emulsification and viscosity reduction energy; Stable emulsions can be produced when the injection rate is greater than 0.3ml/min and the water-oil ratio is range from 6:4 to 8:1. As the temperature increases, the contribution ratio of activated water to EOR decreases. And when the concentration of activated water reaches 1500mg/L, the EOR growth tends to be stable.

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Ion-Tuned Water - An Image-Based Pore-scale Study of Oil Recovery Improvement

Author: Artur Shapoval[1]

Co-authors: Yudong Yuan [1]; Yuzhu Wang [1]; Sheik Rahman [1]

[1] *University of New South Wales*

Corresponding Authors: wangyuzhu2103418@163.com, sheik.rahman@unsw.edu.au, y.yuan@unsw.edu.au, a.shapoval@student.un

Altering calcitic rocks surface properties by means of modifying the composition of injected water (ITW) has gained significant attention in the petroleum industry due to its potential cost-effectiveness. Different mechanisms for the wettability improvement by ITW have been proposed, however, their effects are not quantified and hence it's not possible to know the dominant mechanism responsible for individual reservoir rock and fluid condition. In this work, we propose an innovative method to analyse the experimental data of ion-tuned water flooding with the aid of micro-CT imaging. First, two brines (sulphate enriched brine SW4SO4 and calcium depleted brine SW0.25Ca) were screened based on surface forces study of 100% pure calcite. Next, we perform a set of core-flooding experiments on Austin Chalk samples using seawater for secondary recovery and ITW for tertiary recovery. At the end of each recovery step, high resolution microtomography imaging was carried out to estimate the contact angle and saturation of each phase. The dry images helped us to extract the pore network models which were then used to calculate the oil saturation in each pore of the saturated images for both samples. Finally, the in-situ calculated contact angle is applied for simulation of relative permeability. Results of this study show that both brines were effective in altering the wettability of the sample towards more water-wet with SW4SO4 showing slightly lower values of contact angle. However, when analysing the recovery improvement, we found that SW0.25Ca was more effective at displacing the oil. This is explained by analysing the pore by pore recovery, as SW0.25Ca has shown increased effect at producing from pores of smaller radius (⊠3μm). Combined analysis of core-flooding logs and pore based displacement from the images suggests that SW0.25Ca attributes to dissolution of calcite which improves connectivity between pores and allows for the production of previously trapped oil in smaller pores.

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Comparative Study of Pore Structure Parameters for Various Rock Samples

Authors: Yixin Zhang[1]; Rouzbeh Ghanbarnezhad Moghanloo[2]; Davud Davudov[1]

[1] *University of Oklahoma*

[2] *Univeristy of Oklahoma*

Corresponding Authors: davud.davudov@ou.edu, yzhb7@ou.edu, rouzbeh.gm@ou.edu

In this paper, we utilize a realistic pore network model obtained from digital rock analysis with a hybrid algorithm and stokes equation to simulate single-phase flow for different lithological rock samples (shale, sandstone, carbonate, limestone). Recently, there has been an increasing interest to exploit unconventional shale resources. However, due to uncertainties associated with pore structure and pore connectivity in shale samples, traditional experimental techniques have not been able to establish viable relations between the pore structure characteristics and the macroscopic rock properties. The digital core analysis and pore network modeling are complementary tools to traditional methods for visualizing, analyzing, and modeling of the unconventional reservoirs. We evaluate realistic geometry and topology of the pore structure in shale samples and justify their poor connectivity.

In this paper, we characterize the pore structure of the Marcellus and Eagle Ford rock samples (6 μm in size) using a stack of 600 contiguous high-resolution SEM images. In addition, we utilize 20 stacks of micro-CT images for various sandstone, carbonate, and limestone samples to determine the difference in their pore structure properties. The specific pore space parameters that were studied here are connected porosity, total porosity, pore and throat radii, geometric tortuosity, and coordination number. Additionally, we identify the relationships among these aforementioned parameters and elaborate on the reasons for the ultra-low permeability of shale samples from a mechanistic point of view.

Our analysis indicate that connected porosity is 1.5% and 1.7% for two shale samples, much smaller

than those of sandstone samples (14% ~ 33.8%), carbonate samples (13.2% ~ 21.1%), and limestone samples (3% ~ 5%). The attributed pore size of shale samples ranges from 0.01μm to 0.1μm, while the effective pore radius size of sandstone, carbonate, and limestone samples ranges from 1μm up to 0.1mm. The absolute matrix permeability computed for two shale samples is around 2 nano-darcy, much smaller than that of the sandstone (0.15 ~ 15 darcy), carbonate (0.1 ~ 5 darcy) and limestone (0.02 ~ 8 darcy). Furthermore, the results suggest that for the studied shale samples, Representative Elementary Volume (REV) is around 5 μm, which is smaller than that of carbonate, limestone, and sandstone samples.
This study demonstrates a new insight into the application of digital images, pore network models, and binarized three-dimensional models to assess and visualize the complex micro-pore structure of heterogeneous reservoir rocks and provide a guidance for accurate prediction of REV for different rock samples.

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A Discrete Fracture-Matrix Model for Pressure Transient Analysis in Multistage Fractured Horizontal Wells with Arbitrarily Distributed Natural Fractures

Authors: Hui Liu[1]; Xinwei Liao[1]; Xuefeng Tang[1]; Xiaoliang Zhao[1]; Lijia Yuan[2]; Juan Zhao[2]

[1] *China University of Petroleum,Beijing*

[2] *No.2 oil production plant of Changqing Oilfield*

Corresponding Authors: liuhuiguige@gmail.com, xinwei@cup.edu.cn, 513849056@qq.com, zxl@cup.edu.cn, 313042627@qq.com, huiliu012@gmail.com

Analysis of transient pressure tests has become a reliable and powerful tool for petroleum engineers to identify and interpret the impacts of the complex fracture network on multistage fractured horizontal wells. Although lots of models have been established in the past decades for unconventional reservoirs, the traditional fracture models such as dual-porosity model, dual-permeability model and stripe fracture model have been proved that they are not suitable for stimulating the complex fracture patterns, especially those with asymmetric hydraulic fractures (HFs) and arbitrarily distributed natural fractures (NFs).

In this study, to overcome the disadvantages of the PTA based on the dual-porosity model, dual-permeability model and the stripe fracture model, a Discrete Fracture-Matrix method based numerical well test model (DFM-WTM) is proposed in this paper to simulate better and to interpret the pressure transient behaviors of the MFHW with arbitrarily distributed NFs. In DFM-WTM, the flexible PEBI grid with an automatic local grid refinement algorithm is used so that it can simulate almost any type of fracture patterns and boundary geometries. Meanwhile, with the use of finite volume method, automatic differential solving techniques, and the introduced discrete operators, our simulation workflow is simplified, leading to the fact that pressure transient behaviors of MFHW with complex fracture networks can be obtained not only accurately but also pragmatically and expeditiously. To correctly analyze the impacts of specific parameters, including different fracture properties of HF and NF of our DFM-WTM, sensitivity analysis is conducted.
Finally, a case study is performed to analyze the properties of complex fracture networks of an actual well, which further demonstrates the reliability and the practicality of our DFM-WTM.

The results show that the MFHW with arbitrarily distributed NFs can be divided into eight flow regimes, including: (1) wellbore storage and skin effect, (2) fracture linear flow, (3) bilinear flow, (4) NF-HF fluid supply, (5) second bilinear flow, (6) formation linear flow, (7) pseudo boundary flow, and (8) pseudo radial flow. Different flow regimes have different features, which provide a good guideline for identifying and interpreting the MFHW with complex fracture networks. Besides, a

"dip" is found in the pressure derivative curve, which is caused by the NF-HF fluid supply. Through the sensitivity analysis, it is found that this "dip" is a quite important signal to identify the impacts of NF-HF fluid supply and to fathom the properties of HFs and NFs, due to the fact that this "dip" can be mainly affected by the number and conductivity of both HFs and NFs.

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Modification of Adhesion Properties of Shale by Dilute Acid Treatment

Authors: Shouceng Tian[1]; Panpan Zhang[1]; Mao Sheng[1]

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

Corresponding Authors: tscsydx@163.com, zhangpanpan0819@126.com

Abstract
As an important alternative for conventional energy sources, shale gas development has been a great success with the wide application of horizontal drilling and multistage hydraulic fracturing. To get high conductivity fracture network and reduce the fracture initiation pressure underground, acidizing technology and supercritical CO2 fracturing were introduced in the development of shale reservoirs. Therefore, it is important to investigate the modification of shale in an acidic environment when acid or CO2 is injected into geologic formations as a working fluid. It has previously been shown that acid fluids can enhance the formation conductivity and decrease the hardness of shale. However, less is known about the effect of dilute acid on the adhesion properties of shale. In the study, shale samples are characterized in detail with advanced analysis. Adhesion properties of shale via dilute acid treatment were revealed by atomic force microscopy (AFM). Results indicate that acid treatment can greatly enhance adhesion forces of the shale surface. After acid treatment, the average adhesion forces show a platform-like growth with an increase in loading force. Through analysis of results from AFM, scanning electron microscopy (SEM), and X-ray diffraction (XRD), we affirm that the enhanced adhesion forces are mainly from increased specific surface area and reduced elastic modulus. The results presented in this work help understand the adhesion properties of shale present in an acidic environment, which have great significance in unconventional resources development.

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Experimental Study on Influence of Peclet number on the Dissolution patterns in rough fractures

Author: Ting Wang[1]

Co-authors: Ran Hu [2]; Zhibing Yang [2]; Yifeng Chen [2]

[1] *Wuhan University, School of Water Resources and Hydropower Engineering*

[2] *Wuhan University, School of Water Resources and Hydropower Engineering*

Corresponding Authors: whuran@whu.edu.cn, csyfchen@whu.edu.cn, 2018102060052@whu.edu.cn

The permeability of rocks and aperture of fractures will change due to dissolution and precipitation when a reactive fluid is injected into open apertures. Here, we injected an unsaturated brine water to transparent analog fractures by mating NaCl crystals with rough epoxy resin fracture. The fluid was injected from the center through a 5mm circle and high-resolution light-transmission techniques was used to directly measure the evolving aperture field during each experiment. A set of experiments were conducted under seven different flow rates from 0.05 -5ml/min (Peclet number ranging from 27-2700) (three replicates for each). Reactive infiltration instability was obviously developed in the fractures and fracture dissolution increased the initial hydraulic apertures with a varying range of 2%–15% for flow rate from 0.05-5ml/min. The monitored pressure data also shows a clear increase of permeability of the fractures accordingly. The results also present that for Pe<162, there are clearly minimal fingering channel formed around the inlet at the very beginning of these experiments in the matrix and then dominant pathways formed, all the fluid prefer the dominant channel and crystals can be found in the matrix where nearly no flow reach. While for Pe>162, smaller channels form only on the periphery and NaCl dissolved evenly around the inlet. The higher the flow rates, the larger the radius of evenly dissolved area. The experiments was also compared to a numerical simulations which describes the whole process of couple of convection, dissolution and diffusion and results show a good agreement with experiments.

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3D modelling of subsurface methane leakage through unconsolidated sedimentary aquifers; implications for environmental monitoring

Authors: Gilian Schout[1]; S. Majid Hassanizadeh[1]; Jasper Griffioen[1]; Niels Hartog[1]; Rainer Helmig[2]

[1] *Utrecht University*

[2] *University of Stuttgart*

Corresponding Authors: smhfba@yahoo.com, rainer.helmig@iws.uni-stuttgart.de, g.schout@uu.nl

Subsurface explorations and exploitations, e.g. related to oil & gas production, can create unintended connections between shallow groundwater and deep reservoirs. Such connections may act as pathways for the upward gas leakage, which may impair groundwater quality, contribute to anthropogenic greenhouse gas emissions, and even cause explosion hazard. It is, therefore, crucial to detect any cases of gas leakage. Typically, this is done by measuring methane concentrations in shallow groundwater or in the soil near the surface. The extent to which such leaks may result in methane emissions at the land surface or elevated methane concentrations in groundwater is expected to depend on a range of factors. Besides the gas flow rate through the leakage pathways, it is also affected by processes that retain some of the gas in the subsurface during its upward migration. These include the dissolution of gas in water and its lateral dispersion in overlying aquifers. Such removal processes may be particularly effective in thick unconsolidated sedimentary systems, where there is significant lateral groundwater flow.
To investigate how such factors affect subsurface methane gas leaks, a 3D numerical model was constructed using DuMux, to simulate flow of two phases (water & gas) and behaviour of two components (H2O & CH4) in a sedimentary aquifer under a range of typical conditions. A sensitivity analysis was carried out to determine the most influential properties by varying values of porous medium parameters, two-phase flow parameters, regional groundwater flow velocities and leakage flux. The results show that for typical leakage fluxes, significant amounts of gas may be dissolved and/or dispersed laterally during upward migration, making it effectively undetectable at surface level or only after long time periods (several decades). Under such conditions, measurements at surface are inadequate for determining the occurrence of subsurface gas leakage.

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Temperature Impact on Micro Structure of Rock based on X-ray Computed Tomography

Authors: Haiyuan Yang[None]; Yongfei Yang[None]; Jun Yao[None]

Corresponding Authors: yaojunhdpu@126.com, yanghaiyuanpro@163.com, yangyongfei@upc.edu.cn

Temperature change affects the underground formations greatly, including two cases, the high-temperature effect on underground formations and the interaction between the high-temperature reservoir and the injection fluid. Temperature change affects the pore structure, the fluid flow and the heat transfer process in porous media, which is important for the development of underground reservoirs. In this study, we obtained digital rocks of sandstone and carbonate which experienced the thermal damage and thermal shock based on the X-ray computed tomography. After the image processing, we characterized the micro-structure and analyze the variation of micro-fractures, pore space and matrix as a function of the temperature. We concluded the mechanism of temperature effect on rocks combining the micro-structures and macro-properties (i.e., porosity and permeability). The results show that after heating treatment, the porosity and permeability of sandstone increase with fluctuations due to the thermal expansion and the recrystallization of minerals with the temperature increasing. After experiencing the thermal shock, the fractures and connected pore space propagate greatly, and the cementation degree of carbonate gets worse. With the temperature decreasing, the contraction of rock becomes more obvious than the rock damage due to the thermal shock.

Key Words: CT scanning, temperature, pore structure, fracture, heat transfer simulation

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Yang, H., Zhang, L., Liu, R., Wen, X., Yang, Y., Zhang, L., Zhang, K., Askari, R. (2019a). Thermal conduction simulation based on reconstructed digital rocks with respect to fractures. Energies, 12(14), 2768.

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Study on Formation Damage Mechanism of a Sandstone Reservoir based on Micro-Computed Tomography

Authors: Zhiyu Wang[1]; Yongfei Yang[1]; Jun Yao[1]; Xinze Li[None]; Yingwen Li[None]; Changfu Liu[None]

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

Corresponding Authors: 845891399@qq.com, yaojunhdpu@126.com, 1069939794@qq.com, yangyongfei@upc.edu.cn, 1037038144@qq.com, 1047971053@qq.com

In the process of oilfield development, serious formation damage is commonly caused by the incompatibility of workover fluid with reservoir rock. So it is particularly important to select the best low-damage workover fluid. In this paper, micro-computed tomography (CT) technology is used to

obtain 2D slices of the core and reconstruct 3D structure. First, water-sensitive and salt-sensitive experiments were carried out on the sandstone of X oilfield. It was found that the maximum damage degree of permeability in water-sensitive test was 57.75%, which was medium strong water sensitive. The maximum value of salt-sensitive permeability damage was 47.77%, and the critical salinity ranged from 14987 to 18869 mg/L. Then, two kinds of workover fluids were used respectively for displacement experiment. The experimental results showed that the permeability damage degree of scheme 1 was 39.33% and that of scheme 2 is 72.48%. CT was performed before and after the injection of workover fluid, and the changes of 2D and 3D pore space were analyzed to quantitatively evaluate the damage degree of pore space in the reservoir. Through CT image analysis, it was found that the workover fluid causes the physical migration of in-situ fine particles, resulting in the sealing of part of the pores, and ultimately leading to the decrease of permeability. This work indicates that the incompatibility of workover fluid and reservoir rock will cause serious formation damage in the development of strong water-sensitive and salt-sensitive reservoirs, which should be avoided as far as possible.

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The construction of multi-scale multi-component pore network model with application in shale characterization

Author: Ke Wang[1]

Co-authors: Yongfei Yang [2]; Jun Yao [3]

[1] *Research Center of Multiphase Flow in Porous Media, China University of Petroleum (East China), Qingdao, 266580, China*

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

[3] *Research Centre of Multiphase Flow in Porous Media, School of Petroleum Engineering, China University of Petroleum (East China)*

Corresponding Authors: yangyongfei@upc.edu.cn, rcogfr_upc@126.com

As typical features of shale reservoir, multi-scale and multi-component bring challenges for the accurate full-size pore structure characterization. With the advancement of digital rock physics technology, digital core and pore network model are now considered important tools for micro-scale modelling of porous media. In this work, multi-scale and multi-component pore network model is constructed to be the basis for shale flow simulation. First, regular pore network model containing two scale pore size spectrums is generated. Subdivide method is used to incorporate nanometer scale pores and throats into micrometer scale network model. The effects of structure parameters, including pore size distribution and organic matter content are analyzed. Second, we develop a framework to construct multi-scale model based on real shale pore structure data. Markov chain Monte Carlo method is used to construct organic and inorganic shale digital model. The superpose algorithm developed previously is performed to establish the two-component shale model, which is the input of pore network model extraction process. During the network extraction, the component information is obtained from partitioned pore space. The geometrical and topological properties of organic and inorganic clusters in pore network models are discussed for different shale samples. Results show that the proposed methods for constructing multi-scale multi-component pore network model are verified against available experimental data.

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A Physics-based Data-driven Model for Waterflooding Profile Control and Water Plugging Performance

Author: Hui Zhao[1]

Co-authors: Wei Liu [1]; Shuoliang Wang [2]; Lin Cao [3]; Yuhui Zhou [1]

[1] *Yangtze University*

[2] *China University of Geosciences, Beijing*

[3] *Institute of Porous Flow & Fluid Mechanics, Chinese Academy of Science*

Corresponding Authors: caolin0110@sina.com, zhouyuhui@hotmail.com, liuwei9346@163.com, wangshuoliang@cugb.edu.cn, zhaohui@yangtzeu.edu.cn

Profile control and water plugging is an important way to enhance oil recovery in waterflood reservoirs. However, how to identify the dominant flow channels between well pairs and make quick predictions for profile control and water plugging is still a challenage for real application. In this work, we proposed a new physics-based data-driven model for profile control and water plugging of waterflooding reservoirs. By solving the mass-material-balance and front-tracking equations with well production data, the wo-phase flow rates and saturation is predicted. Throuhgh history matching, two specific parameters of the data-driven model (the interwell transmissibility and control pore volume) are obtained to characterize the interwell connectivity. Considering the mechanism of profile control and water plugging, combined with experimental evaluation of plugging ability, the change of interwell transmissibility and control pore volume influenced by the injected plugging agent is estimated. Then, the future predictions is calculated by solving the mass-material-balance equation. Compared with traditional numerical simulation method, the proposed method performs computational efficiency by hundreds of times and avoids the complicated geological modeling process. A laboratory study of two-dimensional reservoir was conducted to verify the derived physics-based data-driven model. The results shows that the dynamic predictions of physics-based data-driven model is in consistent with the experiment with profile control. The proposed method was also applied to a heterogeneous double-layer reservoir. The calculated water cut and oil production rate matched well with the reservoir data, and the allocation factors correspond well with the streamline simulation model. The longitudinal profile of the injector is improved and the water cut of producers is also reduced. We also test a real field in which the volume of plugging agent for five injectors are optimized.

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Simulation of polymer flooding of conglomerate reservoir based on digital core

Author: Huiying Guo [1]

Co-author: Hao Zhou [1]

[1] *CNPC Xinjiang oilfield*

Corresponding Author: 379426939@qq.com

Polymer flooding in oil industry is a typical multiphase flow process in porous media. In this research, digital cores of Baikouquan Formation and Badaowan Formation of conglomerate reservoir from Junggar Basin were established. Direct method(VOF method) was used in computational fluid dynamics to simulate the process of polymer flooding based on these digital cores. Three-phase flow process of oil,water and polymer was systematically analyzed. And then,the influence factors and mechanism of polymer flooding of conglomerate were investigated.The change of multiphase distribution,velocity and pressure in conglomerate rock are investigated based on simulation results.The production curve is also derived and discussed. After several simulations on digital core,the impact of micro parameters of conglomerate to polymer flooding is also discussed.

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Evaluating influence factors on phase equilibria calculation of CO2/H2O mixture using the CPA equation of state

Authors: Yiteng Li[1]; tao zhang[1]; Shuyu Sun[2]

[1] *King Abdullah University of Science and Technology*

[2] *King Abdullah University of Science and Technology (KAUST)*

Corresponding Authors: shuyu.sun@kaust.edu.sa, tao.zhang.1@kaust.edu.sa, yiteng.li@kaust.edu.sa

Accurate knowledge of CO2 solubility in formation water plays a significant role in the simulation of CO2 flooding in oil reservoirs and CO2 sequestration in deep saline aquifers, thus placing importance on reliable thermodynamic models that enable to accurately describe phase behavior of CO2-H2O system. One popular association model that has been extensively used for this purpose is Cubic-Plus-Association (CPA) equation of state (EOS), which takes advantage of cubic EOS to describe physical interactions while the Wertheim perturbation theory to account for association effects. Since both Peng-Robinson (PR) EOS and Soave-Redlich-Kwong (SRK) EOS, which are the two most popular EOSs in petroleum industry, were originally developed for hydrocarbon mixtures using experiment critical properties and acentric factor, it is necessary to optimize at least the pure-compound parameters of H2O, or both, and binary interaction coefficients by fitting the experimental data. Clearly, the success of phase equilibria modeling of CO2-H2O mixture by CPA EOS heavily depends on all the above optimized parameters, whose quality rest with numerous factors, such as experimental data, combining rules, optimization methods, etc. In this talk, we will summarize reliable experiment data so far by an exhaustive literature review, given the fact that the experimental data measured by different apparatus and methods exhibit various degrees of uncertainty. Moreover, a variety of combining rules proposed in the literature are tested to compare their influence on the prediction accuracy of CPA EOS. Although a majority of CPA model utilizes SRK EOS to describe physical interactions between molecules, recently PR EOS are increasingly employed as the physical term. We will compare the effects of different physical contributions as well. In addition, both optimization methods and objective functions take an important role in fitting parameters to the experimental data. The performance of different optimization schemes will be discussed and analyzed.

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The Peclet number and viscous ratios impact on the fingering evolution during miscible displacement in rough fractures

Author: Xusheng Chen[None]

Co-authors: Ran Hu [1]; Yang Zhibing [1]; Chen Yi-Feng [1]

[1] *Wuhan University*

Corresponding Authors: whuran@whu.edu.cn, 2015301580321@whu.edu.cn

The two-phase miscible displacement process in fracture involves many production processes, including enhanced oil recovery, carbon capture and storage and contaminant transport. The Peclet number and viscosity ratios significantly affect the stability of the interface between displacing and displaced fluid in rough fractures. To demonstrate how the Peclet number and viscosity control the stability during the miscible displacement, we performed a series of experiments in a transparent rock fracture model over a wide range of viscous ratios (50-1000) by injecting dyed water into glycerol solutions at different flux (0.01-10ml/min). The nonlinear finger interactions and four different kinds of fingering mechanism such as splitting, spreading, shielding and coalescence are observed in these experiments. The results show that the interface of fluid-fluid is stable at the early time and gradually develop into fingering as time increasing while the experiment was conducted at low Peclet number and viscosity ratios. However, the nonlinear fingering will immediately form when the Peclet number and viscosity ratios are both high. The experimental results further indicate a transformation mechanism between diffusion and convection during the miscible displacement. A study of transversely and longitudinally one-dimensional concentration profile is presented to demonstrate the mixing zone broaden and the accumulation of mass. Fractal dimension is also calculated to investigate the morphological characteristics of miscible displacement in a rough fracture.

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Analysis of Factors Affecting Fracturing and Absorbing Parameters in Tight Reservoir

Author: Zhu Jiamin[None]

Co-authors: Wu Minglu ; Chen Xianchao

Corresponding Authors: w97612@163.com, chenxianchao2005@126.com, z18020090@s.upc.edu.cn

Abstract: At present, the development of tight oil mostly adopts horizontal well multi-fragmentation fracturing technology. The recently developed non-returned clean fracturing hydraulic fluid retains the reservoir for a long period of time, tends to zero damage to the reservoir, and is conducive to the promotion of spontaneous infiltration Oil and water replacement. The pilot test of tight reservoirs in foreign countries has verified the effectiveness of the production of muddy wells without returning fracturing fluid. However, there is still no effective optimal design method for the design parameters of the infiltration scheme. This paper mainly considers the geological and fluid characteristics of tight oil reservoirs, and establishes a numerical simulation model for fracture-matrix reservoirs in vertical wells and horizontal wells in tight reservoirs during fracturing and infiltration. In the model, the effects of osmosis and surfactants are mainly considered. The effects of natural fracture permeability, matrix porosity, fracturing fluid injection volume, well-removal time, cluster spacing, and crack spacing on the effect of non-return fracturing and wicking were studied. The simulation results show that: The best natural fracture permeability and well-inspiratory time are the best. The greater the porosity of the matrix, the injection volume of the fracturing fluid, the more effective the fracturing and infiltration effects are. When the pressure crack cluster spacing and crack spacing are set at a reasonable value, the suction effect will be the best. Among the above factors, the natural

fracture permeability and the matrix porosity have a greater influence on the infiltration effect, and other parameters will have an impact on the infiltration effect, but the effect is not obvious in the first two.

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Silica nanoparticle-stabilized CO2 foam generation in sandstones

Authors: Ijung Kim[1]; Chun Huh[2]

[1] *Hongik University*

[2] *The University of Texas at Austin*

Corresponding Authors: chunhuh@mail.utexas.edu, ijung.kim@hongik.ac.kr

As the advances in nanoparticle synthesis enabled generation of stable aqueous dispersion of nanoparticles under high temperature and salinity conditions, the effective use of nanoparticles in oilfields becomes a growing research topic. In the enhanced oil recovery, the application of nanoparticles brought more attention to the nanoparticle-stabilized foam generation to increase the volumetric sweep efficiency. Therefore, more fundamental study on nanoparticle-stabilized foam generation is required to explore the untapped area in the enhanced oil recovery.
In this study, surface-modified silica nanoparticles (NPs) with two different surface coating coverage (70% and 100%) were tested for CO2-in-water foam generation in the high pressure core flood experimental setup. A 0.5% suspension of 5–nm-diameter silica NP was prepared in 8.53% NaCl and 1.11% CaCl2 and co-injected with CO2 to the Boise (3900~6200 mD) and Berea (200~500 mD) sandstones with CO2:water of 3:1 by volume. The system pressure was maintained 2200~2300 psi and temperature was kept at 67˚C.
In the Boise sandstone, the silica NPs with 100% surface coating coverage was associated with lower apparent viscosity of the CO2-water mixture, suggesting less viscous foam generation with the higher surface-modified nanoparticles. In the Berea sandstone, however, NP filter cake was formed on the core at the injection side with 70% surface coating, whereas no NP filter cake was observed with 100% surface coating. In the low permeability rock such as Berea sandstone, it is critical to keep a higher NP stability as well as the desirable hydrophilic-CO2-philic balance to generate vigorous foams for a long period. The results suggest a tradeoff between stability and foam formation, where higher surface coating nanoparticles are the most stable but produce weaker foams.
The effect of nanoparticle size on CO2-in-water foam generation was also investigated in Boise sandstones. Four different silica nanoparticle size (5, 12, 25, and 80 nm) were tested under the same conditions as above. Smaller nanoparticles, especially with 5 nm nanoparticles, resulted in vigorous and strong foam generation with greater increase in apparent viscosity of CO2-water mixture in the sandstone, due to quick adsorption on CO2-water interface preventing further coalescence of CO2 foams. Also, a hysteresis in foam viscosity was obvious as the flow rate was decreased. Such a behavior could support the likelihood of stronger foam generation as it goes further from wellbore. The appropriate selection of nanoparticle size and surface coating could lead to the substantial improvement in the enhanced oil recovery.

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An accurate method for the core-scale investigation of in-situ emulsification impact on oil recovery from porous media

Authors: Zheyu Liu[None]; Yiqiang Li[1]

[1] *China University of Petroleum-Beijing*

Corresponding Authors: liyiqiang@cup.edu.cn, zheyu.liu@cup.edu.cn

Unlike microemulsion or emulsion flooding where the emulsion is directly injected into the reservoirs, in other classes of CEOR process, chemicals in the form of surface active materials are carried by water into the reservoir and under reservoir flowing conditions emulsifies oil, i.e. in-situ emulsification. There is no wondered that emulsification has benefits in improving oil recovery. However, there is still lack of effective means to quantitative evaluate the contribution of in-situ emulsification on the oil recovery. In the present study, we (i) develop an approach to mimic in-situ emulsification in porous media, and (ii) investigate the contribution of upstream formed emulsion to the downstream oil displacement at the core scale.
Each experiment includes two cores. The first core is fully saturated oil and conducted water flooding to create different remaining oil saturations. Then surfactant polymer solution is injected into the first core to emulsify remaining oil. The effluent is collected and directly injected into the second core. The residual oil saturation of the first core can be known via chromatography. Then oil volume in emulsions can be easily determined. Moreover, another contrast experiment is performed with the same procedure but keeps the effluent completely demulsification using centrifuge. Mark

separated oil phase and inject aqueous phase to the second core. The post-surfactant polymer flooding is conducted 0.5 PV for the both second cores to remove trapped emulsions. By comparing the incremental recovery factor between two second cores, the performance of emulsified oil from the first core on the incremental recovery factor of the second core can be investigated. The remaining oil saturations of the first core can be manipulated to investigate the effect of oil-water ratio of emulsion to the ultimate recovery factor.
This method succeeds involving two main processes of in-situ emulsion formation: remaining oil peeled off from rock surface and snapped-off when it flows from pores to throats. Results shows the effect of in-situ emulsion on oil recovery depends on the intensity of oil droplets and oil-water ratio in the emulsion. The incremental recovery factor increases as oil-water ratio increasing before it reaches the inverted point, i.e. O/W emulsion can achieve the optimal incremental recovery factor of 4.5% at the oil-water ratio of 4:6 compared to no emulsification. But it significantly decreases as oil-water ratio increasing after it reaches the inverted point (W/O). More trapped emulsion in the porous media cannot be displaced.
Results of the present study provide accurate method to mimic emulsion formation in the pore media and suggest that the emulsion intension and emulsion type should be taken into account in the design of surface-active agents for CEOR.

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Application of GIS and Remote Sensing in Landuse Land Cover Change Detection: A Study of District Malakand, Pakistan

Author: Muhammad Yasir[1]

Co-authors: Hui Sheng [1]; Sami Ur Rehman [2]; Atif Zafar [3]; Muhammad Ilyas [2]; Asif Mehmood [3]

[1] *School of Geosciences, University of Petroleum Qingdao, Qingdao 266580, China*

[2] *Department of Environmental Sciences, University of Peshawar, Peshawar 25120, Pakistan*

[3] *School of Petroleum Engineering, China University of Petroleum Qingdao, Qingdao 266580, China*

Corresponding Authors: alopiyaz1@yahoo.com, atif_zafar1984@yahoo.com

The district Malakand has observed a surprising expansion in growth and developmental activities during previous two decades. The land use pattern has changed drastically because of the expanding population. This study aims to assess different land use land cover changes in the study area between 1996 –2016 using remote sensing and GIS techniques. In this study the Landsat images used were which obtained from the images database of United States Geological Survey (USGS) and vector data was derived from a topographic sheet of the study area. The data were analysed using ArcGIS bands composition and other image enhancement techniques. Images are classified using supervised maximum likelihood classification. Accuracy assessment was carried out through confusion matrix. Results have shown that the vegetation cover is increased by 14% followed by built-up area increased by 6% in previous two decades. However, the water body is decreased by 1%. The Barren land is decreased by 21% in past twenty years. The current study analysis and findings highlights important policy implications for the sustainable LULC management in District Malakand.

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Research on Spread of Crude Oil in Reservoir Based on Porous Media Flow Simulation

Authors: Lei Yang[None]; Bowei Liu[None]

Co-authors: Enhui Sun ; Mo Zhang ; Jun Wu

Corresponding Author: liubw5@cnooc.com.cn

In recent years, porous media flow simulation has been widely used in the study of microscopic remaining oil. In the Bohai Sea, some oilfields that have been developed for many years have entered the stage of high water cut and high recovery. The analysis of reservoir remaining oil and tapping potentials have become a new direction to improve oil recovery. In CFD oilfields with strong bottom water reservoirs, 81% of production wells have reached 90% water content. The analysis of groundwater and crude oil flow in pores is the premise of microscopic residual oil research. In this paper, the casting thin sections are processed in MATLAB environment, core skeleton is extracted by watershed algorithm, and two-dimensional pore network model is constructed by boundary tracking algorithm. Lattice Boltzmann method was used to simulate porous media flow, LBGK model was used to simulate single-phase fluid flow, and Shan-Chen model was used to simulate multi-phase flow. In the pore network model, the bounce-back boundary condition is used to describe the inner boundary of the rock gap, the non-equilibrium extrapolated boundary is used to define pressure (density) inlet/outlet boundary condition. The iterative calculation of the flow simulation in the rock pores is programmed in the C ++ environment, and the visual analysis of dynamic flow is implemented in the software PARAVIEW. The boundary of the porous medium is described by using casting thin sections in the production reservoir. The pores are filled with oil, and water flows into the porous medium from the inlet. Carry out steady-state velocity field analysis and oil-water distribution under different production pressure drop conditions. The simulation results show that when the production pressure drop is low, the proportion of pores participating in the flow (velocity $>$ 0) is 34%, and when the pressure drop increases, this ratio rises to 53%. At this time, 95% of the effluent fluid is water. Further increasing the production pressure drop, the proportion of pores participating in the flow increased to 60%, the extent of water flooding increased, and more oil was further produced. Based on the simulation results, a well with a water content of 97% was selected for trial. A larger oil production was obtained by scaling up the pressure drop. The water content decreased to 96%, and the daily oil production increased from 300 barrels / day to 700 barrels / day.

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Analysis of Hydrate Seafloor Subsidence Induced by Depressurization in Nankai Trough, Japan

Authors: 淑悦丁[None]; 淑霞李[None]; 迪迪武[None]; 爽李[None]

Corresponding Author: s19020146@s.upc.edu.cn

Gas production from hydrate-bearing sediment by depressurization will result in the changes of its porosity, permeability, pore pressure, effective stress and cementing strength, which will reduce the shear strength and bearing capacity of the hydrate sediments. As a consequence, the possible geohazards could cause, such as wellbore instability, submarine landslide, and seafloor subsidence. Given this, taking the first hydrate depressurization in the Nankai Trough of Japan in 2013 as an example, the THMC coupling model using vertical well by depressurization was constructed. The model considers the coupling effect, including hydrate dissociation and formation, heat conduction, convection, and mechanical behavior of hydrate-bearing sediments. The numerical simulation software CMG-STARS was applied to solve the problem and made historical macthing. The evolution

rules of reservoir temperature, pore pressure, stress and seafloor subsidence trend during depressurization were revealed. The effects of the depressurization mode and production pressure difference, permeability, rock properties, the initial formation pressure of stratum subsidence on formation were further studied. The results show that the decrescence of reservoir pressure controls the increase in effective stress and strata subsidence around the production well. The maximum subsidence is located around the production interval, with a settlement of 0.085m. The settlement of the formation decreases rapidly with extending to the reservoir. The production pressure difference increases by 1.5MPa or the initial formation pressure increases by 1MPa, the seafloor settlement increases by 0.02m. The permeability increases by 10 times or the thermal expansion coefficient increases by 1000 times or the young's modulus decreases by 1000 times, the seafloor settlement increases by nearly one time or even more.

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Multi-scale 3D/4D imaging of the pore network in shales and its evolution under subsurface conditions

Authors: Lin Ma[1]; Kevin Taylor[1]; Patrick Dowey[1]; Michael Chandler[2]; Peter Lee[3]

[1] *University of Manchester*

[2] *Universtion of Manchester*

[3] *University Colledge London*

Corresponding Authors: peter.lee@ucl.ac.uk, mike.chandler@manchester.ac.uk, lin.ma@manchester.ac.uk, patrick.dowey@manchester.ac.uk, kevin.taylor@manchester.ac.uk

Pore network variation and evolution are critical factors influencing the generation, storage and transport of hydrocarbons in shale reservoirs and also control the safety of carbon storage and nuclear waste disposal. Combining X-ray tomography and 3D electron microscopy provides a powerful tool for multi-scale imaging and quantification of microstructural information in heterogeneous shales. With this combined approach, pores, organic matter, inorganic mineral phases and fractures can be visualized at six length scales over five orders of magnitude (voxel size 44 μm, 13 μm , 0.8 μm , 100 nm, 10 nm and 0.3 nm).
Samples were selected from several shale basins in Europe and America with variable compositions and properties representing the microstructural diversity observed in shale rocks. Organic matter becomes an interconnected network when organic matter content in selected region increases to a value between 6-18 wt.%. The whole pore network comprises a globally-connected system between phyllosilicate mineral grains (diameter: 6-50 nm), and locally-clustered connected pores within porous organic matter (diameter: 200 - 800 nm). Meanwhile, the dynamic changes of the microstructures are visible at micro-scale using synchrotron-based time-resolved X-ray tomography (4D imaging). Three examples are given in this study: the organic matter maturing with temperatures from 20 to 400℃; the fracture propagation under Vickers indentation; and the mineral precipitation and dissolution under brine conditions.
In summary, multi-scale 3D/4D technique can image shale features leading to a greater understanding of the pore network variation and dynamic change in shales. We use our data to demonstrate the applications under different subsurface conditions and improve the understanding of sedimentological characterisation, burial history, energy extraction and environmental solutions.

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A novel upscaling procedure for characterising heterogeneous shale porosity from nm- to mm-scale in 3D and 4D images

Authors: Lin Ma[1]; Patrick Dowey[1]; Ernest Rutter[1]; Kevin Taylor[1]; Peter Lee[2]

[1] *University of Manchester*

[2] *University Colledge London*

Corresponding Authors: kevin.taylor@manchester.ac.uk, patrick.dowey@manchester.ac.uk, peter.lee@ucl.ac.uk, ernie.rutter@manchester.ac.uk, lin.ma@manchester.ac.uk

Microstructures and pore systems in shales are key to understanding the role of shale in many energy applications. This study proposes a novel multi-stage upscaling procedure to comprehensively investigate the heterogeneous and complex microstructures and pore systems in a laminated and microfractured shale, utilizing 3D multi-scale imaging data. Five imaging techniques were used for characterisation from sub-nanoscale to macroscale (core-scale), spanning four orders of magnitude. Image data collected using X-ray tomography, Focused Ion Beam, and Electron Tomography techniques range in voxel size from 0.6 nm to 13 µm.
Prior to upscaling, a novel two-step analysis was performed to ensure sub-samples were representative. Following this, a three-step procedure, based on homogenising descriptors and computed volume coefficients, was used to upscale the quantified microstructure and pore system. At the highest resolution (nanoscale), four distinct pore types were identified. At the sub-micron scale equations were derived for three pore-associated phases. At the microscale, the volume coefficients were recalculated to upscale the pore system to the macroscale (millimetre). The accuracy of the upscaling methodology was verified, predicting the total porosity within 7.2 % discrepancy compared with helium porosity after five scales. The results provide a unique perspective to understand heterogeneous rock types, breaking though prior scale limitations in the pore system.
Meanwhile, synchrotron-based time-resolved XCT (4D) was applied on the deformation, fracturing, flow behaviors and mineral precipitation and dissolution in shales. These dynamic 4D images further allowed these behaviors to be upscaled from nm-scale to mm-scale or cm-scale.

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Analysis of Neural Networks Performances for Flux Regression in Discrete Fracture Networks

Authors: Stefano Berrone[1]; Francesco Della Santa[2]; Sandra Pieraccini[None]; Francesco Vaccarino[2]

[1] *Politecnico di Torino, Italy*

[2] *Politecnico di Torino*

Corresponding Authors: stefano.berrone@polito.it, sandra.pieraccini@polito.it, francesco.dellasanta@polito.it

Many engineering applications, like fossil fuels extraction and analysis of water resources in the underground, need to characterize flow and transport through fractured media in the subsurface of the soil with accurate simulation models. However, there is a lack of full knowledge of these sparse systems of fracture networks and, therefore, only a statistical representation of them can be given. In this context, the systems of underground fractures and the flow and transport simulations of fluids are performed via Discrete Fracture Networks (DFNs).
Since DFNs are stochastically generated, both with respect to geometrical properties and hydrogeological properties, thousands of DFN generations and simulations must be considered to characterize flow in a real fractured medium; therefore, in order to speed up simulation processes and to build

alternative model reduction methods, it is worth considering the application of Neural Networks (NNs) for flux regression 1.
In this work, following 1, the application of Neural Networks to flux regression problems in a DFN is considered, showing the multitask architecture adopted for this framework; then, the behavior of the regression quality is analyzed with respect to both the size of the training set and the intrinsic properties characterizing the DFN considered.

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Lattice Boltzmann Modeling of the Apparent Viscosity of Thinning-Elastic Fluids in Porous Media

Authors: Chiyu Xie[1]; Matthew Balhoff[1]

[1] *The University of Texas at Austin*

Corresponding Authors: chiyu.xie@gmail.com, balhoff@mail.utexas.edu

The flow of non-Newtonian fluids in porous media is important in many engineering applications such as filtration processes, water treatment and oil recovery. Many of these non-Newtonian fluids exhibit combined rheological complexities, such as a thinning-elastic fluid with both shear-thinning and viscoelastic behaviors1. Steady shear measurements by laboratory rheometers only show the shear-thinning behavior of a thinning-elastic fluid, however, many experiments at the core scale have also shown strong thickening behavior in porous media at high shear rates2. Experiments using microchannels have also been performed to discover the thickening mechanisms of viscoelastic fluids[3]. Most of the existing studies explained observations of thickening as due to extensional viscosity[4].
In this work, we aim at discovering more pore scale insights of the thickening behavior of the thinning-elastic fluids in porous media at higher shear rates. A hybrid lattice Boltzmann (LB) model is developed. It applies the Oldroyd-B constitutive equation and the Carreau model, respectively, to account for the viscoelastic and shear-thinning behaviors of the thinning-elastic fluid in porous media. Both of the viscoelastic and the shear-thinning features of the model are verified against analytical solutions, which shows excellent agreement.
The apparent viscosity of the thinning-elastic fluids flowing through porous media with periodically stacked cylindrical grains are calculated. The thinning-then-thickening viscosity curve of the thinning-elastic fluid observed in experiments is reproduced by the present pore-scale simulations. In addition to the traditional extensional theory, we propose other important mechanisms for the increase of apparent viscosity of viscoelastic fluids at higher shear rates. These include the reduction of conductivity due to stagnant fluid, the compressed effective flow region and larger energy dissipations caused by the viscoelastic instability. We also find that the viscoelastic thickening effect is more prominent in porous geometries with a large pore-throat ratio.

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Oil Recovery Characteristics of Supercritical CO2 Huff-n-Puff Process in Ultra-Low Permeable Porous Media

Authors: Dongxing Du[1]; Yinjie Shen [2]; Di Zhao[2]; Weifeng Lv[3]; Ninghong Jia[3]; Tong Li[3]; Yingge Li[4]

[1] *Qingado University of Science and Technology*

[2] *Qingdao University of Science and Technology*

[3] *RIPED, PetroChina*

[4] *15066857079@126.com*

Corresponding Authors: jianinghong@petrochina.com.cn, lweifeng@petrochina.com.cn, 1764469690@qq.com, du-dongxing@vip.163.com, tongl886@petrochina.com.cn, myzhaodi@163.com

Cyclic CO2 stimulation, aka "CO2 huff and puff injection', has been effectively applied to improve oil recovery in tight formations. With three stages of huff (injection), soaking, and puff (production), CO2 huff-n-puff process could assure sufficient solubility between CO2 and crude oil to recover extra oil from tight reserves. To guide successful field applications of this technique, corresponding laboratory works are substantial.

In this paper, four rounds of supercritical CO2 huff-n-puff process are performed under system pressure of 28MPa and temperature of 65℃ to investigate the oil recovery characteristics in extra-low permeable cores (diameter of 5cm, length of 5cm and oil phase permeability around 0.01mD). Nuclear Magnetic resonance (NMR) tests are also performed to reveal the harvesting mechanism in the tight medium for each round of operation based on T2 spectrum. To show the advantage of the CO2 huff-n-puff process, four rounds of carbonate water huff-n-puff process are also carried out together with NMR tests.

Experimental results show that,
1) Supercritical CO2 huff and puff process has obvious oil recovery effect. In the first round operation, the oil production rate can reach to 33.53%, while in the subsequent rounds, the oil production rate gradually reduces to 11.86%, 7.85% and 2.3%, indicating three rounds of operation could be performed to obtain satisfactory oil recovery. The NMR test results show that the first CO2 huff and puff can even drive the oil phase into smaller pores, and most of the oil recovery phases are ultimately contributed by the larger pores of the core, and there are still some oil remaining in the smaller pores after four rounds of huff and puff process.
2) Carbonated water huff and puff process has certain oil recovery effect. In the first round of operation, the oil production is the highest of 19.14%, while in the subsequent rounds, the oil production rate is gradually reduced to 9.57%, 5.74% and 1.84%, indicating two rounds of carbonated water huff and puff process could be tried for better oil recovery. NMR results show that the first huff and puff process mainly produces the oil phase in larger pores, while the second, third and fourth huff and puff process could drive oil out from smaller pores as well.

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A new making method of artificial core through changing epoxy resin form

Authors: Kun Xie[1]; Kaoping Song[2]; Xiangguo Lu[1]; Bao Cao[1]; Jian Hou[3]; Wei Lin [4]; Jinxiang Liu[1]; Weijia Cao[1]; Cheng Su[1]

[1] *Northeast Petroleum University*

[2] *China University of Petroleum(Beijing)*

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

[4] *University of Chinese Academy of Sciences*

Corresponding Authors: luxiangguo2008@163.com, 1543284194@qq.com, 859232711@qq.com, xiekun725@163.com, 380500259@qq.com, 973838044@163.com, cbjh091@126.com, 369499907@qq.com, sichuandexuesheng@163.com

In recent years, artificial core cemented by quartz sand and liquid epoxy resin has been widely used in petroleum science researches at home and abroad. However, the liquid epoxy resin used in the making process of artificial core will cause obvious differences in pore throat structure between artificial core and natural core. The differences in core pore throat structure will become more obvious with the decrease of permeability. Therefore, this paper conducted the researches on a new making method of artificial core through changing epoxy resin form, aiming at the two problems that the core inner heterogeneity for the liquid epoxy resin is difficult to distribute evenly on the surface of quartz sand, and the failure contact cementation between and sand particles for the sand surface coated by epoxy resin. First, the high-purity linear epoxy resin, phenolic resin , 2-methylimidazole, acrylate and conventional epoxy defoamer were used to prepare the heat curable epoxy resin powder, the curing temperature is about 180℃. And then, the new making method of artificial core was established by using mixing method of solid cementing agent and solid core structure materials(solid heat curable epoxy resin powder and the mixing material of quartz sand and clay mineral). The reservoir water was added during the mixing process of solid cementing agent and solid core structure materials to eliminate the influence of air on the pressing process. Finally, the core structure was characterized by permeability testing, analysis of casting piece and high pressure mercury injection, and the comparative analysis with common artificial core was also done. The artificial cores prepared by new making method has the characteristics of inter particle contact cementation that conventional artificial core making method cannot achieve, well homogeneity in core inner structure, environmental materials , simple and efficient production process. The new type artificial cores can be used in the field of geotechnical engineering and petroleum engineering to conduct experimental study on the flow mechanism of porous medium.

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Flow behavior of CO2/ N2/ CH4 huff and puff process for enhanced heavy oil recovery

Authors: Wu Mingxuan[1]; Zhaomin Li[1]; Songyan Li[1]; Chen Lu[1]; Zhengxiao Xu[1]

[1] *College of Petroleum Engineering, China University of Petroleum (East China),*

Corresponding Authors: 1248520980@qq.com, mingxuanwu@126.com

In this paper, experimental techniques have been utilized to research heavy oil properties containing different concentrations of viscosity reducer in three gases (CO2, N2, CH4) huff-n-puff processes under reservoir conditions. The results show that the total oil recovery after the fifth (CO2/ N2/

CH4) cycle of huff-n-huff processes is CO2>CH4> N2 under the same conditions. Five cycles of huff-n-puff were carried out to study the changes of recovery and the composition of the produced oil in each cycle. The viscosity and asphaltene content of produced oil is lower than that of the original oil. However, with the increase of huff-n-puff cycles, the content of asphaltene increased. The gas-oil change rates of the three gases during the huff-n-huff were calculated. Under the existing experimental conditions, the order of the gas-oil change rate in the first cycles from high to low is CH4> N2 > CO2. As the cycles increases, the gas-oil change rate decreases rapidly. The state of foam oil produced by the three-gas throughput experiment was experimentally tested. The foam oil in the produced oil is compared. The micro-glass model was used to study the flow morphology of foamy oil in simulated porous media during pressure reduction. On the basis of microscopic visualization experiments of the heavy oil with different gases dissolved, the foamy oil microflow characteristics were researched

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Geothermal Simulation Using MRST

Authors: Øystein Klemetsdal[1]; Marine Collignon[2]; Olav Møyner[3]; Halvor Nilsen[1]; Odd Andersen[1]; Knut-Andreas Lie[1]

[1] *SINTEF Digital*

[2] *Unversity of Geneva*

[3] *SINTEF, NTNU*

Corresponding Authors: oystein.klemetsdal@sintef.no, olav.moyner@sintef.no, odd.andersen@sintef.no, knut-andreas.lie@sintef.no, halvormoll.nilsen@sintef.no, marine.collignon@unige.ch

Thermal energy from medium to high-enthalpy aquifers is an appealing energy resource: it is renewable, always on, and, at least in principle, available anywhere on the planet. Moreover, and perhaps equally important, aquifers are excellent candidates for flexible large-scale energy storage. This is imperative in order to transition from a mostly fossil-based energy supply to a mixture of renewable energy from multiple temporal resources (e.g., solar and wind power). Efficient utilization of geothermal heat requires a solid knowledge of the local subsurface situation and reservoir properties, including factors such as energy efficiency, storage capacity, economical aspects (e.g., drilling and operational costs), and compliance with legal regulations. This complexity can only be properly understood through numerical simulations. However, state-of-the-art numerical simulation tools for geothermal applications are somewhat lagging behind simulation technology for other subsurface applications (especially for oil and gas), even though they describe systems governed by the same physical principles.

In this work, we present a module for geothermal simulation in the open-source MATLAB Reservoir Simulation Toolbox (MRST). The implementation is based on the industry standard finite volume discretization with single-point upstream evaluation and two-point flux approximation, and can therefore benefit from powerful solvers widely used by the reservoir simulation community. Moreover, the module can be integrated with well-established functionality from petroleum applications that are already part of MRST, such as optimal well control, inverse modelling, and uncertainty quantification, and apply it to real geomodels using complex fluid physics. We demonstrate the applicability of the module on a number of cases, ranging from simple conceptual tests, to realistic high-temperature aquifer thermal energy storage (HT-ATES) systems with industry-grade complexity.

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Study on electrokinetic reactive fluid in dielectric porous media with Lattice Boltzmann Method

Authors: Haijing Li[1]; Herman Clercx[1]; Federico Toschi[1]

[1] *Department of Applied Physics, Eindhoven University of Technology*

Corresponding Authors: f.toschi@tue.nl, h.j.h.clercx@tue.nl, h.li@tue.nl

Packing structures are applied in many chemistry reactors to enhance the reaction conversion rate by increasing the reaction interface or working as catalyst. To better understand the interplay among the packing structures, fluid property and reaction efficiency, experiments can be carried out. However, direct measurements are costly or difficult to perform especially for electrokinetic flows. In this aspect, numerical simulation may represent a valuable tool. In this work, we present results obtained by a 2D Lattice Boltzmann (LB) model that we developed to qualitatively study the electrokinetic fluid in a packed dielectric porous media chemistry reactor featuring electric breakdown reactions. In this model, we solve a combined set of equations, namely: the Navier-Stokes equations for the momentum field, the advection-diffusion and the Nernst-Planck equations for electrokinetics, and the Poisson equation for the electric field. This model allows us to study the dynamical interaction of the fluid density, velocity, concentration and electric field. Primary result shows that the dielectric packing beads will locally enhance the electric field, therefore, influencing the reaction rate of the electric breakdown reaction, see Fig. 1. We will show results when adopt rectangular packing beads. Because of the sharp edges, different influence on the local electric field will be expected when different orientations of the beads are applied, see Fig. 2. Finally, we also show how higher electric field and the highest reaction efficiency can be achieved by optimising the orientation of the beads.

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Hydrophobicity/Hydrophilicity Driven CO2 Solubility in Kaolinite Nanopores in Relation to Carbon Sequestration

Authors: Wenhui Li[1]; Zhehui Jin[1]

[1] *University of Alberta*

Corresponding Authors: wenhui4@ualberta.ca, zhehui2@ualberta.ca

Carbon capture and sequestration (CCS) is an urgent mission for human beings due to the increasingly severe climate change. Storing CO2 in depleted oil or gas reservoirs is a viable option to reduce the amount of CO2 released to the atmosphere. In this process, the solubility of CO2 in finely-grained nanoporous media may play an important role to determine the storage amount. In this study, we use molecular simulation (MD) to study the effects of surface wettability on the CO2 solubility in nanopores under typical geological conditions (373 K and up to 400 bar). Kaolinite is chosen as the target nanoporous media due to its abundance in the strata with two naturally different basal surfaces (hydrophilic and hydrophobic ones, respectively). Compared to the bulk solubility, CO2 over-solubility in 2-nm pores is observed under the hydrophobic confinement, while under-solubility is seen under the hydrophilic confinement. From the microscopic view, in hydrophobic nanopores, CO2 and water have co-adsorption on the kaolinite surface, while CO2 has more prominent layers than water. In addition, CO2 molecules align parallel to the surface in the adsorption layers. The strong CO2 adsorption at the nanopore surface is the dominant mechanism inducing "over-solubility". However, in hydrophilic nanopores, water forms strong adsorption layers at the surface, which repels CO2 molecules. Also, CO2 presents a perpendicular orientation to the water film. As a result, CO2 has an under-solubility in the hydrophilic nanopores. Our work should provide important insights into the CO2 solubility in a confined environment and the effects of surface wettability, which may play a crucial role in the optimization of geological carbon sequestration.

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Effects of Salinity and N-, S-, and O-Bearing Polar Components on Light Oil-Brine Interfacial Properties from Molecular Perspectives

Authors: Wenhui Li[1]; Zhehui Jin[1]

[1] *University of Alberta*

Corresponding Authors: zhehui2@ualberta.ca, wenhui4@ualberta.ca

Oil-brine interfacial tension (IFT) is a fundamentally important property in, but not limited to, the oil recovery process and oil-brine separation. Reducing oil-brine IFT to an ultra-low value (10-2~10-3 mN/m) can drastically reduce the residual oil saturation. In addition, oil-brine IFT also significantly affects the working efficiency of demulsifiers, during the oil-brine separation process. However, the effects of salinity on oil-brine IFT have been much of debate in the past from both experiments and modeling studies. Besides, the effects of commonly present polar components (N-, S-, and O-bearing compounds) in the oil phase on oil-brine IFT are rarely studied. Therefore, in this work, we use molecular dynamics (MD) simulations to study the oil-brine interfacial properties by designing seven systems containing different oil compositions (decane with/without polar component), and brine salinity up to ~14 wt%. We carefully investigate the salinity and polar component effects by analyzing IFT, density profiles, orientation parameters, hydrogen bonds, and charge distributions. The results indicate that O-bearing compounds (phenol and decanoic acid) can significantly reduce the oil-brine IFT, and exhibit the highest Gibbs surface excess relative to water, while the others, including N-bearing compounds (pyridine and quinoline) and S-bearing compounds (thiophene and benzothiophene), only slightly decrease the oil-brine IFTs and show a relatively small Gibbs surface excess. Increasing salinity can slightly increase the oil-brine IFT except the system containing phenol which presents a decrease. Phenol and decanoic acid have a preference to be perpendicular to the interface and generate numerous hydrogen bonds with water in the interfacial region, while others prefer to be parallel to the interface with much fewer hydrogen bonds with water. On the other hand, salinity has a marginal effect on the orientation of polar molecules and hydrogen bond number in the interfacial region. The charges at the interfaces on the brine and oil sides are negative and positive, respectively, and the polar components disturb the arrangement of water molecules in the interfacial regions, while adding salt ions result in the higher peak values of charges in terms of

water and system. Our study should provide some new insight into the oil-bine interfacial issues and clarify some unsettled disputes.

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Viscosity of hydrocarbons in slit pores by molecular dynamics

Author: Vasily Pisarev[1]

Co-author: Nikolay Kondratyuk [1]

[1] *National Research University Higher School of Economics*

Corresponding Author: pisarevvv@gmail.com

We study the viscosity of liquid hydrocarbons in slit pores with atomistic structure using a non-equilibrium molecular dynamics method. The pore walls are described by ClayFF force field, which allows us to study the slip behavior under shear. We consider pores in pyrophilite and montmorillonite with widths from 2 to 10 nm.

The non-equilibrium molecular dynamics simulations are made by applying a constant force to each hydrogen atom in hydrocarbon. That simulates a constant pressure gradient along the pore, and a Poiseuille velocity profile is established as a result. From the velocity profile and known external force, we get the viscosity coefficient and estimate the slip length.

We observe the increase of viscosity of liquid in pores, compared to the bulk phase of the same density, with the stronger effect in narrower pores. We also see that the slip length is low, so that in practical applications no-slip boundary conditions must be adequate for the description of flow.

The abstract was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE) and supported within the framework of a subsidy by the Russian Academic Excellence Project '5-100'.

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A New Approach to 3D Imaging of Multi-scale Pore Systems in Carbonates using Confocal Microscopy

Author: Ahmed Hassan[1]

Co-authors: Viswasanthi Chandra [1]; Maxim Yutkin [2]; Tadeusz Patzek [1]

[1] *KAUST*

[2] *King Abdullah University of Science and Technology*

Corresponding Authors: ahmed.hassan@kaust.edu.sa, viswasanthi.chandra@kaust.edu.sa, maxim.yutkin@gmail.com, tadeusz.patzek@kaust.edu.sa

Microporous carbonates host a significant portion of the remaining oil-in-place in the giant carbonate reservoirs. For example, intragranular microporosity in carbonates is usually surrounded by large pores that provide efficient flow bypasses and make oil recovery from the microporous grains very difficult. In this work, we use confocal laser scanning microscopy (CLSM) to produce high-resolution 3D images of the pore space to characterize and quantify the multi-scale pore types and their interconnectivity.

In this work, we critically review the main challenges involved in confocal image acquisition and signal processing to obtain the high-resolution 3D images of the micropore space. We follow the protocol described in our earlier study (Hassan et al., 2019) to fabricate epoxy pore casts of microporous carbonate rock samples. After dissolving the rock grains with HCl, we use CLSM to produce 3D images of the fluorescent epoxy conformed to the pore space of the rock sample. We evaluate different imaging conditions to optimize the quality of the pore cast imagery with respect to various experimental factors including the choice of fluorophore, objective lens and medium of imaging. Furthermore, we experimentally measure the resolution for the confocal imaging system to ensure our pore cast images capture the realistic geometric attributes of the rock pore space. We determine the "true"resolution by evaluating the Point Spread Function (PSF) from imaging standard sub-resolution fluorescent microspheres. We demonstrate that the deviations from the theoretical values of the resolution, which can be as high as 60% in some systems, are common since the true resolution depends on imaging optics, sample geometry, signal-to-noise ratio, and dynamic range of the detector.

We applied our protocol to characterize a standard limestone sample and were able to identify a bimodal porosity distribution at lateral and axial resolutions of 1 μm and 9.2 μm, respectively. Moreover, we visualized the sub-micron scale 3D interconnectivity between macro- and micro-pores at lateral- and axial-resolutions of 0.36 μm and 2 μm, respectively, as shown in Figure 1. The high-fidelity 3D images of the pore space allowed for a more reliable petrophysical interpretation and prediction of transport properties, as we verified the estimated values for porosity, pore-size distribution, and permeability with experimental measurements.

The imaging methodology we have developed in this study can be used as a standard protocol for obtaining high-quality 3D images of epoxy pore casts using confocal microscopy, and can contribute to improved characterization of micritic carbonate reservoirs and oil recovery methods therein.

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A Microfluidic Investigation of In-Situ Water-in-Oil Emulsion Formation during Waterflooding of Heavy Oil Reservoirs

Author: Mohammad Salehpour[1]

Co-authors: Zahra Sakhaei [1]; Hassan Mahani [2]; Masoud Riazi [1]

[1] *Enhanced Oil Recovery (EOR) Research Center, IOR/EOR Research Institute, Shiraz University, Shiraz, Iran*

[2] *Department of Chemical and Petroleum Engineering, Sharif University of Technology, Azadi Street, Tehran, Iran*

Corresponding Authors: mriazi180@gmail.com, zahra.sakhaei71@gmail.com, hmahani@sharif.edu, mohamad.salehpour@gmail.com

In-situ emulsion formation in porous media generally occurs naturally or by adding chemicals such as surfactants. In natural emulsion formation, the reaction between basic and acidic functional parts of crude oil components may generate surfactants at the water/oil interface 1. These naturally induced surfactants create emulsions by encapsulating the dispersed liquid through a dense interfacial film and will be stabilized by asphaltenes molecules 2. Unpredictable oil recovery, oil viscosity increment, formation damage, pressure fluctuations, and additional separation difficulties are among the significant problems of emulsion formation. In order to address the aforementioned complications, micro-scale assessments using microfluidic chips can help gain an in-depth understanding of the involved factors on emulsion flow.

In this paper, the impact of the displacing phase salinity and flow rate on the severity of in-situ water-in-oil emulsion formation were investigated through microfluidic experiments. A heterogeneous glass micromodel with an average pore and throat size of 590μm and 155μm respectively was utilized for micro-scale experiments. An asphaltenic heavy crude oil and synthesized NaCl brines were used as the oleic and aqueous phases, respectively. Waterflooding experiments were performed for three brine salinities (2800, 5600 and 56000 ppm) at two flow rates (0.01 and 0.1 cc/min).

The results show that water snap-off, water shortcut, and emulsion division are the principal mechanisms forming in-situ water-oil-emulsion during heavy oil displacement. When the injection water enters the pore space, due to the high capillary pressure at the throat entrance, it splits into small discontinuous drops inside the oil phase, which is referred to as water snap-off mechanism. Water shortcut happens when the injected water stream gets in contact with connate water film and tends to flow in a narrow pathway of connate water. Moreover, a macro emulsion in a pore can be separated into two smaller discontinuous water drops that flow inside and with the oil phase through throats; thereby causing emulsion division. These phenomena are responsible for excess in-situ emulsion formation. Observations indicate that stable emulsions formed in porous media show viscoelastic behavior. In the case of low injection rate, pressure spikes, which are effectuated by emulsions and further pore blockage, are observed throughout the tests. Low injection rate could increase the interactions between the basic and acidic functional groups of the crude oil with brine, and as a result, surfactants intensifying emulsions stability are generated at the water/oil interface. The results suggest that the injection of water with the lowest interfacial tension and viscoelasticity corresponding with the lowest brine salinity (NaCl 5600 ppm) result in the largest pressure instabilities due to extensive water snap-off.

The results of this study provide novel insights into the various mechanisms of water-in-oil emulsion, and have direct implications for the application of low salinity waterflooding and other water-based EOR methods in heavy oil recovery.

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Implementation of ePc-SAFT Equation of State into MRST Compositional for Modelling of Salt Precipitation during CO2 Storage in Saline Aquifers

Authors: Mohammad Masoudi[1]; Saeed Parvin[2]; Rohaldin Miri[3]; Helge Hellevang[4]

[1] *University of Oslo, Department of Geosciences*

[2] *Petroleum University of Technology*

[3] *Iran university of science and technology*

[4] *Department of Geosciences, University of Oslo*

Corresponding Authors: helge.hellevang@geo.uio.no, mohammad.masoudi@geo.uio.no, saeed.parvin.20@gmail.com, rohaldinmiri@iust.ac.ir

Global warming results in the climate change that has fatal consequences for all the specious of the planet Earth including humans. The main cause of global warming is the emission of greenhouse gasses. According to United States Environmental Protection Agency (EPA), carbon dioxide (CO2) accounts for 76% of global greenhouse gasses 1. Carbon capture and sequestration (CCS) is a relatively new technology that can capture CO2 from its major sources before it reaches to the atmosphere and safely store it under the ground (deep saline aquifers or depleted oil and gas reservoirs). To maximize safety and cost-efficiency of CO2 storage, it is necessary to understand how a high permeability in the near-well region is maintained. Salt precipitation driven by the evaporation of formation water into under-saturated (dry) super-critical CO2 stream is the main reason of the injectivity loss in the context of CO2 storage in saline aquifers.
To model formation drying-out and subsequent halite-precipitation, we implemented an advanced, accurate, and reliable fluid model, ePC-SAFT [2,3] into MATLAB reservoir simulation toolbox (MRST). ePC-SAFT effectively takes into account various type of molecular interactions, such as the effect of ionic (salts) and associative molecules (CO2 and water). Injection of dry CO2 into a brine-saturated core-scale domain is simulated and sensitivity analysis over various parameters are performed. We show that the new model is capable to quantitatively represent the physics of salt precipitation under different reservoir conditions.

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Flow of sub- and supercritical CO2 in nano-porous ceramics: direct comparison of laboratory experiments and numerical simulation

Authors: Steffen Nolte[1]; Yue Wang[2]; Reinhard Fink[1]; Bernhard M. Krooss[1]; Moran Wang[2]; Alexandra Amann-Hildenbrand[1]

[1] *RWTH Aachen University*

[2] *Tsinghua University*

Corresponding Authors: alexandra.amann@emr.rwth-aachen.de, reinhard.fink@emr.rwth-aachen.de, mrwang@tsinghua.edu.cn, wangyue14thu@163.com, bernhard.krooss@emr.rwth-aachen.de, steffen.nolte@emr.rwth-aachen.de

Transport processes of carbon dioxide (CO2) in micro- and nanoporous rocks are of potential relevance in various geotechnical contexts such as carbon capture and storage (CCS), enhanced oil recovery (EOR) or fracturing of gas and oil shales. These transport processes are typically controlled

by fluid-dynamic (e.g. slip flow) and rock mechanic (pore compressibility) effects. Temperatures and pressures of many relevant applications are around the critical point of CO2 (304.25 K, 7.39 MPa).
While numerous modeling approaches have addressed various aspects of gas transport in micro- and nanoporous media, there is a notorious shortage of reliable experimental data to validate or verify the modeling results. Major issues are uncertainties regarding the experimental starting and boundary conditions and material properties (pore size distributions, mechanical properties etc.). Recent studies (Fink et al., 2017) have shown that interpretations of transport mechanisms in low-permeable rocks are still controversial. In order to reduce the complexity encountered in natural rocks flow experiments and simulations should first focus on synthetic, homogeneous and well-defined porous media. The "NanGasPor"project has been initiated to establish a direct link between modelers and experimentalists side in order to create feedback and improve the match between experimental data and numerical models.
In this context a series of flow tests with different gases has been conducted on sintered ceramic (α-Al2O3, >99%) discs with a homogeneous pore network and a narrow pore-throat distribution. All experiments were conducted at 35℃ i.e. slightly above the critical temperature of CO2. Helium pycnometry, low-pressure nitrogen adsorption (BET) and mercury intrusion porosimetry (MIP) were used for a comprehensive characterization of the pore system of the specimens. The porosity is 29% with the most prominent pore diameter of 70 nm, as determined by BET and MIP. The ceramic material is very rigid and chemically inert. Pure fluid-dynamic effects can thus be investigated without interference of poro-elastic deformation and adsorption phenomena.
The permeability measurements were performed with different gases (H2, He, N2, Ar, CH4, CO2) at pressures ranging from 0.2 to 30 MPa using steady state and non-steady state techniques.
Characteristic slip flow effects in terms of a linear dependency of apparent permeability coefficients (kapp) and reciprocal mean pressure (Klinkenberg trend) were observed in all tests. Intrinsic permeability coefficients determined from these trends range around 25 μD (2.5•10-17 m2). While the Klinkenberg trends of the other gases were essentially linear, the tests with CO2 exhibited increasing positive deviations from the trend around the critical pressure of 7.39 MPa. This coincides with the dramatic density increase of supercritical CO2 in this pressure range, which is also strongly affected by small temperature variations. The flow experiments were evaluated using the Span-Wagner (1996) equation of state (EoS) for CO2, which is considered the most accurate EoS presently available. Numerical modeling is being conducted to investigate the limitations of the experimental approach and the effects of temperature and pressure.

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Spectral induced polarization of calcite precipitation: 2D experimental pore scale observation

Authors: Satoshi Izumoto[1]; Johan Alexander (Sander) Huisman[2]; Egon Zimmermann[1]; Yves Méheust[3]; Francesco Gomez[3]; Hervé Tabuteau[4]; Joris Heyman[4]; Romain Laniel[5]; Harry Vereecken[2]; Tanguy Le Borgne[6]

[1] *Forschungszentrum Jülich*

[2] *FZ-Juelich (Juelich Research Centre), Germany*

[3] *Géosciences Rennes*

[4] *CNRS*

[5] *Université de Rennes 1*

[6] *University of Rennes*

Corresponding Authors: joris.heyman@univ-rennes1.fr, s.izumoto@fz-juelich.de, h.vereecken@fz-juelich.de, yves.meheust@univ-rennes1.fr, romain.laniel@univ-rennes1.fr, tanguy.le-borgne@univ-rennes1.fr, e.zimmermann@fz-juelich.de, francesco.gomez@univ-rennes1.fr, s.huisman@fz-juelich.de, herve.tabuteau@univ-rennes1.fr

Induced calcite precipitation is used in geotechnics to modify the mechanical and hydrological properties of the underground. It is also being considered to remediate soil contaminated with heavy metals. Previous studies have shown that spectral induced polarization (SIP) can be used to monitor calcite precipitation. However, the results obtained so far are not consistent, and the processes that generate the SIP response are not clear. This study aims to improve the understanding of how calcite precipitation generates SIP response in porous media. For this, a 2D cell with a porous medium was developed that allows to visualize the dynamics of calcite precipitation while making SIP measurements. Calcite precipitation was generated by injecting Na2CO3 and CaCl2 solutions through two inlet ports for 76 hours. The development of precipitation in the region where the two solutions mixed was monitored with a camera. Calcite crystal growth was observed with a high-resolution camera at selected locations. The SIP response was measured in three regions of the cell. The results from image analysis indicated that calcite precipitation occurred at the interface of the two injected solutions in a narrow zone that developed along the mixing interface in the first 16 hours. Most of the calcite precipitation occurred in this period, but the SIP response did not show significant changes in this period. After 16 hours, calcite precipitation occurred in an even narrower zone that resulted in a wall that slowly increased in thickness in vertical direction, and the SIP response started to increase up to a phase shift of 90 mrads in this period. Additionally, the frequency of the peak phase was higher for the region near the injection, which is commonly interpreted as a smaller crystal size. However, observations indicated that the size of calcite crystals was almost constant in the entire mixing zone. In a next step, SIP measurements were simulated with a finite element model using the shape of the mixing zone with calcite precipitation and a non-polarizing background solution as in the experiment. The simulation results indicated that the strength of the polarization depends on the continuity of the wall. Furthermore, it was found that the peak frequency can vary with position even with homogeneous electrical properties of the calcite due to the heterogeneous distribution of the calcite precipitation. Both findings are consistent with the observed results. It was also found that the observed increase in SIP response after 16 hours in the experiment is likely related to an increase in chargeability associated with calcite precipitation. However, it is still an open question why a small increase in the height of the calcite precipitation resulted in a strong increase in the SIP response. Overall, our experiments indicated that the SIP response does not necessarily represent the total mass of calcite precipitation in the measurement region. Instead, the SIP response was controlled by pore scale processes and the spatial position of the calcite precipitation. This highlights the importance of understanding pore scale processes for the interpretation of the SIP response of calcite.

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Experimental study of non-Newtonian behavior of foam flow in very high permeability porous media

Authors: Sagyn Omirbekov[1]; Hossein Davarzani[2]; Stéfan Colombano[2]; Azita Ahmadi-Sénichault[3]

[1] *BRGM (French geological survey); Institut de Mécanique et Ingénierie de Bordeaux (I2M, TREFLE), Arts et Métiers ParisTech*

[2] *BRGM (French geological survey)*

[3] *Institut de Mécanique et Ingénierie de Bordeaux (I2M, TREFLE), Arts et Métiers ParisTech*

Corresponding Authors: s.omirbekov@brgm.fr, s.colombano@brgm.fr, h.davarzani@brgm.fr, azita.ahmadi@ensam.eu

The study of foam flow in porous media has mostly been related to the oil industry, especially for Enhanced Oil Recovery (EOR) techniques. More recently, foam has also been used in soil remediation processes for several targets. For instance, as a pollutant sweeping fluid 1, as a vectorization fluid

to transport soil cleaning additives or gases [2, 3]. However, porous media in soil remediation cases are often highly permeable and unconsolidated, contrary to the oil industry. Moreover, in-situ foam generation in aquifers is doubtful due to the big size of the pores, leading to low capillary pressures. Consequently, foam flow in aquifers calls for further investigation.

Understanding of foam flow in porous media is hindered by the complicated behavior of foam, which is also the subject of many contradictions in the literature. For example, in previous studies, foam in porous media was indicated to behave as a non-Newtonian fluid with various rheological behaviors: shear-thinning [4], shear-thickening 5, yield stress fluid [6], or dependent upon the foam quality (foam gas volume fraction) [7]. Some authors also considered foam to behave as a yield stress fluid when flowing in porous media modeled as a bundle of capillary tubes [8, 9]. However, it must be noted that most studies presented in the literature are related to low permeable porous media for EOR applications.

The main objective of this investigation is to determine, experimentally, the rheological behavior of pre-generated foam, particularly in very high permeable unconsolidated porous media. Besides, this study aims to collate the outcome with experimental results of foam flow in capillary tubes and bulk foam surveys using a rheometer, thereby to explore the pre-generated foam using different methods.

In order to embody the concept, two packed columns filled with fine sand and 1 mm glass beads respectively are used to generate foam by co-injection of N2 and a surfactant solution. The pre-generated foam has been injected in calibrated glass beads packed columns (4 cm internal diameter, 40 cm length) with various total flow rates and liquid/gas volume fractions (foam qualities) to investigate the apparent foam viscosity. For a given foam quality, the effect of flow rate on the apparent viscosity of foam in the column was examined. To study the effect of foam generator (bubble size) on the apparent foam viscosity, the pre-generated foam with a fixed foam quality was injected into a 1 mm glass beads packed column with various values of total flow rate. Also, the rheology behavior of pre-generated foam was experimentally investigated in capillary tubes and in bulk foam case using a rheometer.

As a result, foam flow in porous media was showed to feature a non-linear behavior, and the apparent viscosity was found to fit the Herschel-Bulkley model. We found that the foam flow behavior in high permeable porous media and in capillary tubes are consistent with the rheology behavior of bulk foam. These insights can guide the study of pre-generated foam in very high permeable porous media, especially for application in soil remediation processes.

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Effect of solute mixing on non-linear reaction kinetics

Authors: Charlotte Le Traon[1]; Kate Maher[2]; Tomas Aquino[3]; Tanguy Le Borgne[4]

[1] *Université de Rennes 1*

[2] *University of Stanford*

[3] *IDAEA – CSIC*

[4] *University of Rennes*

Corresponding Authors: tanguy.le-borgne@univ-rennes1.fr, kmaher@stanford.edu, tomas.aquino@idaea.csic.es, charlotte.le.traon@gmail.com

Subsurface environments are biogeochemical reactors characterized by a range of chemical gradients, such as: gradients of dissolved oxygen in the unsaturated zone, gradients of electron donors and acceptors in the hyporheic zone, gradients of chemical compounds in contaminated sites, gradients of groundwater age and dissolved species in catchments. Yet, effective reaction kinetics are generally estimated from batch reactors, i.e. zero gradient conditions. Here we investigate the effect of chemical gradients on the average kinetics of fluid-mineral reactions. We focus on non-linear reactions, where the reaction rate is a non-linear function of local concentrations, where the power law exponent is related to the reaction stoichiometry. In this common situation, the effect of chemical gradients on reaction kinetics is expected to be particularly important. We combine reactive transport models with solute mixing theories to establish effective fluid-mineral kinetics, and relate them to mixing rates. We compare the resulting kinetics to those of homogeneous systems for a range of Damköhler numbers in order to investigate the respective roles of reaction and mixing processes.

We first consider the case of a diffusing pulse of reactant in a homogeneous velocity field evolving under the action of diffusion and reaction with the mineral phase. The resulting spatially and temporally variable chemical gradients lead to power law kinetics for the average reaction rates, with exponents that differ from those of batch reactors. Solute mixing is found to either accelerate or slow down the average reaction kinetics, depending on the local kinetic laws. We derive approximate analytical solutions for the evolution of concentration distribution in time and space allowing us to predict the effective reaction kinetics resulting from the non-uniformity of the concentration field. In a second step, we investigate the effect of mixing in heterogeneous permeability fields on reaction kinetics, using CrunchFlow simulations. The enhancement of mixing resulting from plume stretching is shown to affect the scaling of the mean reaction rate with the mean concentration. We discuss the link between the flow heterogeneity and the average reaction kinetics. These results open new perspectives to understand and model coupled mixing and fluid-mineral reactions in heterogeneous media.

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Facilitating visualization and analysis of time-resolved X-ray micro-CT data using sliding widow reconstruction and flip point detection

Author: Marijn Boone[1]

Co-authors: Jan Dewanckele [1]; Arno Merkle [1]; Tom Bultreys [2]; Tim De Kock [2]

[1] *TESCAN*

[2] *Ghent University*

Corresponding Authors: tom.bultreys@ugent.be, tim.dekock@ugent.be, marijn.boone@tescan.com, jan.dewanckele@tescan.com, arno.merkle@tescan.com

Time-resolved X-ray micro-CT imaging is rapidly emerging as an essential technique to understand materials evolution, facilitating in situ investigation in porous materials like deformation, crystal growth and fluid flow. The push toward time-resolved dynamic 3D imaging has been spearheaded by synchrotron radiation facilities, with temporal resolutions going below one second. Recent advances in laboratory-based X-ray micro-CT imaging are pushing achievable temporal resolutions from hours down to seconds, enabling real-time imaging of dynamic processes.
Time-lapse and dynamic X-ray micro-CT imaging generates a vast amount of projection data and 3D reconstructed volumes which require further post processing. Devising the right workflow strategy prior to reconstruction is essential to quickly identify the interesting moments in time and space and helps to reduce the amount of data that is generated. Here we present two methods for facilitating the analysis of dynamic processes using time-resolved X-ray micro-CT data: sliding window reconstruction and flip point detection. In time-lapse micro-CT imaging, the set of 3D volumes is predefined by the number of individual scans or rotations that is performed. Movement of the sample during one of these individual scans will result in image artefacts and blurring in the affected reconstructed volumes. Instead, by using a dynamic imaging approach, where an uninterrupted series of projections is acquired while the sample is continuously rotating, one can enable significantly more flexibility in reconstruction and allows one to tune the reconstruction windows to pinpoint the movement and reduce motion artefacts in a given reconstruction. This 'sliding window' approach is illustrated using an in situ drainage process, where pore filling events are pinpointed in time and the time steps just before and after the pore filling are analyzed. Further analysis on reconstructed datasets using flip point detection or automated detection of voxel changes through time is also presented. Instead of analyzing the reconstructed 3D images individually, we directly incorporate the time dimension within the 3D analysis flow, by analyzing grey value changes of individual and clusters of voxels though time. This enables automatic pinpointing of changes inside the volume in time and space, with substantially less calculation overhead and time investment and greater flexibility compared to conventional post-3D reconstruction evaluation approaches (e.g. comparison of segmented volumes). We illustrate this by using a limestone weathering process, where we link the dissolution processes of the calcite rock matrix with crystallization of gypsum crusts on the sample.

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The impact of surface roughens on contact angle hysteresis studied by molecular dynamics simulation

Authors: Wei Yong[1]; Yingfang Zhou[2]; Jos J. Derksen[1]

[1] *Univeristy of Aberdeen*

[2] *University of Aberdeen*

Corresponding Authors: yingfang.zhou@abdn.ac.uk, r01wy18@abdn.ac.uk, jderksen@abdn.ac.uk

Contact angle defined at three phase contact line plays a critical role in amount of process, for example hydrocarbon recovery process and subsurface groundwater flow and it is one of the essential parameters required to model these process at pore scale. Contact angle hysteresis has been observed both at lab and numerical simulations, and it is analysed based on instinct contact angle measured on smooth solid surface. While surface roughness is observed in natural surfaces at all length scales (Garrison, et al. 1991) and it is one of the most important surface property that affects the surface wetting behaviour (Yaghoubi and Foroutan 2018, Khan and Singh 2014, Park and et al. 2011). And thus, it should be challenged to quantify contact angle hysteresis based on equilibrium contact angle measured on smooth surfaces (Hazlett 1992).

In this study, we performed a detailed molecular dynamic (MD) simulation (all the simulations are conducted with the open source MD code - LAMMPS) study on the impact of surface roughness on equilibrium contact angle and the hysteresis between advancing and receding contact angles. We first studied the equilibrium contact angle of water nanodroplets on regular, e.g., pillars-, holes- and ridges-structured, and generated gaussian random rough surface. The results on these rough surfaces are explained by either Wenzel (Wenzel 1936) or Cassie (Cassie and Baxter 1944) model. Consistent with previous studies (Yaghoubi and Foroutan 2018, Khan and Singh 2014), our results also shows that for all the structured surfaces, there exists a critical height beyond which water droplets can transit for the Wenzel state to the Cassie state. The results also show that the contact angle of droplet increase with surface roughness. In addition, we analysed the impact of water droplet size on the rough surface wetting and the water molecular distribution and its adsorption phenomena at liquid-solid interface in both Wenzel and Cassie state through water concentration profile along the direction normal to the surface. The dynamic contact angle and hysteresis between advancing and receding contact angle is studied by applying the body force on the nanodroplet after the droplet reaches static equilibrium over pillared surface with a schematic of MD simulation. Our primary results show that hysteresis could be enhanced with increasing surface roughness.

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Gas Slippage in Partially Saturated Tight Rocks

Authors: Steffen Nolte[1]; Mohammadebrahim Shabani[2]; Reinhard Fink[1]; Bernhard M. Krooss[1]; Alexandra Amann-Hildenbrand[1]

[1] *RWTH Aachen University*

[2] *University of Calgary*

Corresponding Authors: steffen.nolte@emr.rwth-aachen.de, alexandra.amann@emr.rwth-aachen.de, bernhard.krooss@emr.rwth-aachen.de, reinhard.fink@emr.rwth-aachen.de

Gas slippage is a well-known effect during gas flow in narrow pores/capillaries (Kundt & Warburg, 1875; Klinkenberg, 1941). While it has been intensely studied for single-phase gas flow, only few

experimental studies have investigated gas slippage in two-phase (gas/liquid) flow systems as encountered e.g. in tight gas reservoirs (Jones & Owens, 1980; Sampath & Keighin, 1982; Reinecke & Sleep, 2002; Li & Horne, 2001; Rushing et al, 2003). These reservoirs contain connate/irreducible water or imbibed water after drilling and hydraulic fracturing. Investigation of gas slippage in these two-phase systems is therefore essential for the prediction of gas production rate from tight reservoirs (Li & Horne, 2001).

We have investigated the influence of water on gas flow using sample plugs in the dry state and after moisture-equilibration at three defined levels of relative humidity (33%, 53%, 75% RH). Porosity values, determined by means of helium pycnometry and saturation/buoyancy (Archimedes method), ranged from 3.4 to 12.6%. Permeability measurements were performed with helium using steady state techniques.

Apparent effective gas permeability coefficients were below 10-16 m^2 (0.1 mD) and decreased by up to three orders of magnitude with increasing water content. Above a critical water saturation level, effective permeability coefficients depend on drainage- and imbibition-controlled re-distribution of the water phase. Below this critical level apparent permeability coefficients are predominantly controlled by slippage effects. As the slip factor is inversely proportional to the transport pore diameter, an increase in slip factor indicates decreasing mean effective transport pore sizes. In the literature this is attributed to the deposition of water films on the pore walls ("funicular flow", Dullien, 1992; Li et al., 2018). In contrast, decreasing slip factors are interpreted to result from flow in a separate network of larger gas-filled pores ("channel flow", Dullien, 1992) as the smaller capillaries are occupied by the wetting phases (water).

To avoid saturation gradients within the samples, flow tests must be conducted with low gas pressure gradients, either with controlled back-pressure in the steady-state mode or as non-steady state experiments. Apparent gas permeability may also be determined from gas uptake experiments (Cui et al, 2010; Peng et al., 2016; Yang et al., 2016; Gaus et al., 2019). These tests can be conducted under different controlled stress conditions in combination with porosity measurements. Here drainage effects are negligible and water saturation can be assessed at elevated pore pressures.

The complex set of different processes (slip flow, drainage/imbibition, and poro-mechanical responses) acting simultaneously and with partially antagonistic effects can be analyzed by systematic variation of starting and boundary conditions and by applying specific evaluation strategies.

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Multi-scale diffusion mechanism of coalbed methane in coal and new diffusion model of dynamic diffusion coefficient

Authors: zhiqiang LI[None]; jiansong Peng[None]

Corresponding Authors: 1039308044@qq.com, maximos2004@126.com

In order to solve the problem that classical diffusion model cannot accurately fit full-time gas diffusion process in coal particle, gas diffusion in coal particle experiments were carried out under various conditions by use of typical coals in china. The results calculated by classical diffusion model show that experimental values of diffusion ratio are greater than the theoretical value before some time, however, the former is less than the latter after that time. The law is certain. The classical diffusion model cannot precisely fit full-time gas diffusion process and the error is great, and then the special phenomenon for diffusion coefficient decreasing with increasing time was found. The new physical model of multi-scale pore distributing in coal was put forward. Base on new model, we assumed that pore distribution within coal is heterogeneous and multi-scale, and has self-similar fractal structure, which causes multistage distribution of diffusion coefficient within coal and determines macroscopic diffusion mechanism of gas. From the surface to the center of coal, the pore distributes from big to small and diffusion coefficient decreases from large to small accordingly. Gas diffuses rapidly from big pore of large diffusion coefficient in the early and slowly from small pore of small one in the late until micro pore is influenced in the end. The multilevel diffusion coefficient distribution caused by multi-size pore results in diffusion mechanism of diffusion coefficient deceasing with increasing time. According to the assumption, two parameters, initial diffusion coefficient (D0) and decay coefficient(β), were introduced to reflect decay characteristic of dynamic diffusion coefficient. The mathematic model of dynamic diffusion coefficient was put forward. The new model, verified by 200 datas, can fit full-time process of gas diffusion in coal under various conditions. Meanwhile, the new model covers the classical unipore diffusion model and bidisperse one and generalizes the latter ones. The new model can explain the problems caused by classical one, and on the accuracy, simplicity, explanatory and predictability, is better than the bi-disperse model and empirical equations. The new model provides the new algorithm for researchers to determine the coalbed methane content, reserves and outburst predicting index and to explain diffusion mechanism under various conditions.

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The optimal wettability for oil recovery by waterflooding: dependence on structural factors

Authors: Fanli Liu[1]; Moran Wang[1]

[1] *Tsinghua University*

Corresponding Authors: mrwang@tsinghua.edu.cn, liu-fl17@mails.tsinghua.edu.cn

The wetting condition of the reservoir is known to have a big impact on oil recovery by waterflooding and wettability alteration has generally been accepted as the major mechanism of low salinity waterflooding (LSW), a promising enhanced oil recovery technique. However, there remain unsolved

issues in terms of the optimal wettability for oil recovery. The common belief in LSW studies that altering the rock to a more water-wet condition is better for oil recovery seems to be in contradiction with many coreflooding experiments, where the maximum in oil recovery was found at near-neutral wettability. There were also contradictions between different numerical simulation studies of waterflooding, where the optimal wettability was found to be either neutral, strongly water-wet, or even oil-wet.
One possible explanation for those contradictions is that the optimal wettability is not always the same under all conditions but dependent on the properties of different porous media. In this work, the impact of structural factors on the optimal wettability for oil recovery is investigated by numerical simulation. Two-dimensional porous media are reconstructed from micro-CT images of sandstone. The structures are then modified in different manners and the waterflooding process is simulated in the original and modified structures. Results show that minor changes in the topology can have considerable influences on how wettability impacts the oil recovery and thus the optimal wettability. This can be one reason why different simulation studies found the best recovery in different wetting condition. Finally, the dependence of the optimal wettability on several structural factors is studied and summarized.

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Volumetric response of crushed dunite during carbonation reaction under controlled σ-P-T conditions

Author: Jinfeng Liu[1]

Co-authors: Timotheus Wolterbeek [2]; Christopher Spiers [2]

[1] *1. School of Earth Sciences and Engineering, Sun Yat-Sen University, 510275, Guangzhou, China. 2. Guangdong Provincial Key Lab of Geodynamics and Geohazards, Sun Yat-Sen University, Zhuhai, China. 3. Southern Marine Science and Engineering Guangdong Laboratory, Zhuhai, China*

[2] *Department of Earth Sciences, Faculty of Geosciences, Utrecht University, 3584CD Utrecht, The Netherlands.*

Corresponding Authors: c.j.spiers@uu.nl, t.k.t.wolterbeek@uu.nl, liujinf5@mail.sysu.edu.cn

Naturally, olivine reacts with CO2-rich fluids, producing carbonates and silica. If in completion, this reaction will cause a large increase in the solid volume (~85%), which can generate a significant stress/force when it occurs in a confined space. This may be used to fracture the surrounding rocks in the context of injection of industrially captured CO2 into peridotites for permanent sequestration. Contrarily, this volume-increasing reaction may also clog transport paths and thus inhibit CO2 access, leading to little or no volumetric increase at industrial time scales. Although observations from natural systems suggest that reaction-induced fracturing during peridotite carbonation can occur, the fracturing mechanism has not been experimentally reproduced under in-situ stress-temperature-chemical conditions. Here, we report 9 flow-through experiments performed on pre-compacted Åheim Dunite (containing ~85% olivine) powders (grain size 36-50 μm) during carbonation reaction under controlled σ-P-T conditions. This was done using a purpose-built apparatus, consisting of a flow-through system accommodated with a uniaxial servo-controlled loading system. The experiments were performed at a constant temperature of 150℃ and constant (Terzaghi) effective stress of 1, 5, 15MPa, respectively, using the loading system. Meanwhile, the samples were exposed to CO2 saturated brine (containing 1M NaCl plus 0.64M NaHCO3, pH~3), CO2 saturated water (pH~3), NaHCO3 saturated solution (pH~9) and NaHSO4 solution (pH~3), respectively, and the permeability was measured for all experiments using the flow-through system by means of the steady-state method. Each experiment took 2-4 weeks. The experiments demonstrate that the samples exhibited 0.15-0.37% compaction strain when CO2 saturated brine, CO2 saturated water, and NaHCO3 saturated solution flow through and the sample permeability drops in the order from 10-17 to 10-20 m2. Particularly, compaction strains of the sample exposed to CO2-saturated brine and NaHCO3 saturated solution were larger than 0.29%, suggesting these fluids have a major effect compared to

CO2 saturated water. More importantly, the influence of fluids on the rates of compaction and permeability reduction yields the order of CO2 saturated brine > NaHCO3 saturated solution > CO2 saturated water. This is consistent with the effect of fluids on rates of olivine carbonation reported in the literature. The mass of the samples was also found to increase ~3-5wt%, indicating CO2 was integrated into the crystal structure of the product carbonates. The mechanism responsible for the observed behavior is likely to be that the dissolution of olivine that occurred first at the grain contact surface leads to compaction, followed by precipitation of carbonates at porous that clogs the transport paths and thus reduces the permeability. By contrast, for the NaHSO4 flow-through experiment where no carbonation reaction occurred, the sample permeability increased from 2*10-17 to 7*10-17 m2, associated with 0.05% compaction. In the final, the mass of the sample reduced ~5%. This suggests that magnesium and silica may be partly leached out from the sample. As a result, our current findings suggest that volume increasing precipitation produced via the carbonation reaction under in-situ subsurface conditions will clog transport paths, though the chemical process in the experiments is now performing based on XRD results.

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Multiscale study of natural gas components behavior under nanoconfinement

Authors: Vítor Sermoud[1]; Gabriel Barbosa[1]; Amaro Barreto Jr.[2]; Frederico Tavares[1]; Iuri Segtovich[2]; Jessica Maciel[2]

[1] *PEQ/COPPE/UFRJ*

[2] *EQ/UFRJ*

Corresponding Author: tavares@eq.ufrj.br

Thermodynamic modeling of confined fluids and the study of adsorptive phenomena are essential for several systems of current interest, such as shale gas exploration and the separation process using porous adsorbents. One of the difficulties faced in this type of study is the ability to measure the macroscopic properties of adsorbates within the cavities. We can overcome this barrier with the thermodynamics analysis at different scales.
We can use models that simulate interactions between molecules to obtain the equilibrium and transport properties with high acuity, allowing us to calculate many process parameters. Such as the Henry constant, surface tension, and even adsorption isotherms. The drawback of these molecular simulation methodologies is the high computational cost.
Equations of state are the main chemical engineering tools capable of correlating components in different phases, bringing with them much information about the equilibrium properties that we can use in numerous processes and reservoir simulators. On the other hand, there is still a great effort to produce equations of state that are capable of presenting the behavior of fluid under the induction of an adsorbent structure.
Trying to bring the accuracy of molecular simulation results, but at a lower computational cost, tools derived from density functional theory are developed to treat the different system components as a continuous distribution function. Among the strategies focused on confined fluids, it is worth highlighting the strategies that approach the adsorbent non-locally, and those that describe the solid explicitly.
Here we present a multiscale study to obtain confined fluid properties in some systems of interest. Among them, advances in molecular dynamics studies for calculation of equilibrium and transport properties of natural gas components in barite, calcite, and montmorillonite adsorbents. We also present advances in the application of macroscale models to describe the behavior of natural gas molecules enclosed in the hydrate cavities. In addition, we show comparisons and development of new models. Among them, a comparison between the solutions of the NLDFT, QSDFT models considering the WCA and the DFT-PC-SAFT dispersion term. Also, the development of a thermodynamic adsorption model at compressible matrices, representing matrix swelling and iso-structural

equilibrium phenomena. Moreover, the development of the equation of state with a wall induction term for mesopores and micropores. Finally, a discussion of the discrimination of multiple DFT solutions concerning the value of the grand canonical potential.

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A Study of Plane Water Injection Adjustment and Distribution Technology Using Flow Tube Method

Authors: Ming YANG[1]; Fengjun ZHOU[2]; Yuan LEI[1]; Cunliang CHEN[1]; Yu WANG[1]; Dong MA[1]

[1] *Research Institute of Tianjin Branch, CNOOC Energy Technology& Services Co.*

[2] *Research Institute of Tianyajin Branch, CNOOC Energy Technology& Services Co.*

Corresponding Authors: leiyuan@cnooc.com.cn, madong4@cnooc.com.cn, zhoufj2@cnooc.com.cn, wangyu67@cnooc.com.cn, yangming18@cnooc.com.cn, chencl4@cnooc.com.cn

The irregular well pattern is used in offshore fault block reservoir with complex reservoir boundary. Because the plane heterogeneity is strong, the plane contradiction in the process of water flooding with irregular well pattern will lead to the imbalance of water drive, which affects the development effect of water drive. It is an important way to improve the water flooding effect of fault block reservoir by optimizing the plane injection distribution in order to realize the balanced displacement of reservoir. In this paper, considering the heterogeneity of reservoir and the distribution of injection production streamline of irregular well pattern, focus on production well, the injection and production well group is partitioned into several triangle seepage units. Each unit is divided into numerous flow tubes, and the seepage in each flow tube conforms to Buckley-Leverett water drive theory. The plane sweep coefficient of seepage unit is obtained by using the multi flow pipe method at different time with different oil-water distribution mode. According to the proportion of the Critical Sweep Coefficients (at a certain time the rise of the seepage unit sweep coefficient slow down, the sweep coefficient of the units at that time is called Critical Sweep Coefficient) of seepage units, the plane water injection distribution is calculated with liquid volume of production well. The plane water injection adjustment and distribution technology is established. This study is used to guide the plane adjustment of water injection in block S1 of BZ oilfield in the south of Bohai Sea. And one well group is illustrated as an example in this paper. Through the plane adjustment of water injection, the daily oil increase of the well group is 80m3, water cut decreased 20%, and the effect is obvious. This technology is widely used in block S1. The water content rise rate is 1.3%, and the natural decline rate is only 7.2%, which are all lower than the theoretical level. The technology application effect is good. This technology can be applied to optimize water injection in offshore fault block reservoir and greatly improves water drive development effect.

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Use of limited deep formation monitoring data with shallow aquifer

observations for leakage monitoring in geologic carbon storage

Authors: Tissa Illangasekare[1]; Ahmad Askar[1]; Jakub Solovský[2]; Radek Fucik[2]; Ye Zhang[3]; Jiangyin Jiao,[3]; Andrew Trautz[1]

[1] *Colorado School of Mines*

[2] *Czech Technical University in Prague*

[3] *University of Wyoming*

Corresponding Authors: radek.fucik@fjfi.cvut.cz, atrautz@mines.edu, askar@mymail.mies.edu, tissa@mines.edu, jakubsolovsky@gmail.com, jjiao1@uwyo.edu, yzhang9@uwyo.edu

The storing of carbon dioxide in deep geologic formations is pursued to mitigate global warming. In the case of carbon storage, both during and post-injection phases, it is possible for the formation brine to leak through natural faults, pressure-induced fractures, or failed well casings. Two scientific challenges have to be addressed to safely store the carbon in the deep formation while protecting the shallow aquifers. The first, characterizing the affected geologic formations, and the second is monitoring the leakage. Monitoring involves determining leakage locations and tracking of the brine plume through the geologic formation between the deep confining layer used for storage and the shallow aquifer. Challenges to the characterization derive from the limitations and sparsity of observational data in deep formations. Effective monitoring poses both scientific and engineering challenges as the leakage locations not known, and the resulting pathways cannot be predicted easily. A study is underway to address issues of monitoring and characterizing the geologic formations under scenarios of supercritical CO2 storage and leakage. An approach developed in this study relies on a new inverse theory that integrates limited observational data from deep formations with more abundant or easily obtainable shallow aquifer data. As it is not feasible to obtain data in field systems to verify the developed approach, an innovative set of experiments were conducted in an intermediate scale synthetic aquifer. The processes of leakage and the migration of the brine plume were simulated and accurately monitored using sensors and high spatially resolved aqueous sampling. The conceptual design of experiments and validation of the inversion method are presented. Even though the focus of this study is carbon storage, the findings and tools are applicable to leakage of produced water containing toxic contaminants during hydraulic fracturing.

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CO2 Transport and Mineralization in Reactive Magnesium Cement-Based Concrete

Authors: Afiq Muzhafar Kemis Yahyah[1]; Anna Herring[1]; Fatin Mahdini[1]; Mohammad Saadatfar[2]; Penny King[1]

[1] *The Australian National University*

[2] *Australian National University (ANU)*

Corresponding Authors: anna.herring@anu.edu.au, penny.king@anu.edu.au, mohd.kemisyahyah@anu.edu.au, mohammad.saadatfar@anu.edu.au, u5984455@anu.edu.au

Cements made of reactive magnesium minerals (”reactive magnesium cements”, or RMCs) have been proposed as an alternative to commonly used Portland cement (PC). PC production is a significant carbon emissions source, producing on the order of 5% of the world’s carbon emissions annually [Worrell et al., 2001]. RMC production requires a lower calcination temperature compared to PC (800 vs. 1450^oC), enabling the usage of renewable energy for calcination process; and RMCs necessarily consume significant amounts of CO₂ during cementation [Ruan and

Unluer, 2016]. These factors combined indicate that replacement of PC with RMCs in construction and industrial applications could largely reduce carbon emissions derived from cement production and concrete usage.

Upon initial mixing, RMC-aggregate mixtures are porous and relatively weak, but over time, and with exposure to water and gaseous CO₂, RMCs react to form stable magnesium-carbonate solids within the pore structure of the original aggregate matrix. The formation of carbonate cements strengthens the concrete, but can also clog the pore space and limit complete reaction.

This study reports on a suite of experiments focused on RMC curing in different aggregate compositions, under accelerated and ambient CO₂ concentration conditions. The evolution of the 3D concrete microstructure was characterized using high resolution 3D X-ray computed tomography via the ANU CTLab; accompanying temporally-resolved surface mineral characterization was accomplished using FTIR diffraction spectroscopy. Endpoint chemical composition of samples was determined used X-ray diffraction. The results highlight the importance of designing curing conditions in order to facilitate CO₂ transport and reactions throughout the concrete, and provide insight into options to optimise initial aggregate composition such that the RMCs enhance CO₂ uptake and cement strength.

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Capillarity Dynamics of Spontaneous Imbibition in Porous Media: from Pore Scale to Continuum Scale

Author: Chao-Zhong Qin[1]

[1] *TU/e*

Corresponding Author: c.qin@tue.nl

Spontaneous imbibition plays an important role in many industrial and subsurface applications such as enhanced oil/gas recovery in fractured reservoirs and geological sequestration of carbon dioxide. In those applications, the imbibition rate and the trapping of nonwetting phase are of great interest. To predict spontaneous imbibition by the two-phase Darcy model, a number of material properties need to be determined such as capillary pressure and relative permeability. Moreover, sharp wetting fronts observed in many core-scale experiments indicate that capillarity dynamics in spontaneous imbibition is strong, particularly at its early stage. This challenges conventional measurements of material properties which were mostly conducted in the equilibrium. In this talk, I will first introduce a novel dynamic pore-network model for spontaneous imbibition in porous media. Multiform idealized pore elements have been used to represent complex pore spaces so that our model bears the potential to quantitatively predict spontaneous imbibition for a 'real'porous medium 1. The model is used to understand capillarity dynamics at the pore scale. Then, I will address the upscaling of the pore-scale information to the REV-scale modeling of spontaneous imbibition. Finally, I will summarize the challenges in the REV-scale modeling of spontaneous imbibition in porous media; and further talk about how to include this capillarity dynamics in the two-phase Darcy model.

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Transport of chemotactic bacteria in granular media with randomly distributed NAPL ganglia: Modeling and simulation

Authors: Beibei Gao[1]; Ehsan Taghizadeh[2]; Brian Wood[2]; Roseanne Ford[1]

[1] *University of Virginia*

[2] *Oregon State University*

Corresponding Authors: taghizae@oregonstate.edu, rmf3f@virginia.edu, brian.wood@oregonstate.edu, bg6hp@virginia.edu

Nonaqueous phase liquids (NAPLs), constituted of organic pollutants such as petroleum products, are the most persistent industrial contaminants in natural groundwater aquifers. Conventional treatments leave behind NAPLs in less permeable regions of the formation, where they remain as long term sources of contamination which leach slowly into surrounding groundwater. Components of NAPLs, such as toluene and naphthalene, are slightly soluble in water and confirmed to be attractants for soil-inhabiting chemotactic bacteria. Chemotactic bacteria can detect the presence of chemoattractants, swim toward them, and degrade them for metabolic activities. Therefore, bacterial chemotaxis is a natural process that facilitates the bioremediation of residual NAPL contaminants. Previous studies revealed the tendency for chemotactic bacteria to accumulate near NAPLs under various scenarios. However, the transport of chemotactic bacteria in granular media with discrete NAPL contaminant sources is not well understood. Inspired by an experimental study where chemotactic bacteria invaded a sand column containing NAPL ganglia, we utilized numerical simulations to visualize how bacteria distribute inside the column, especially near the ganglia. An advection-dispersion equation was applied to describe the bacterial transport; for chemotactic bacteria, an additional advective-like term, chemotactic velocity, was incorporated to account for the biased movement toward chemoattractants. We assumed that chemotactic and nonchemotactic bacteria have the same equilibrium sorption coefficient on the sand and kinetic sorption rate on NAPLs. Interestingly, chemotaxis drives bacteria toward NAPL ganglia, which increases their likelihood of sorption. Thus, chemotaxis was expected to yield a patchy distribution and greater overall retention of chemotactic bacteria within the sand column as compared to nonchemotactic bacteria.
Numerical simulation is a convenient tool for providing insight into bacterial transport. Bacterial breakthrough curves exported from our simulations are consistent with experimental observations. In our simulation, NAPL ganglia are randomly distributed in a sand column, and the soluble naphthalene concentration profile gradually increases along the flow direction, except near the locations where the ganglia are fixed. In the presence of chemoattractants, a pulse input of chemotactic bacteria displays localized hotspots with higher concentrations near trapped NAPL ganglia, whereas nonchemotactic bacteria exhibit an expected Gaussian distribution subject to dispersion as it progresses along the length of the sand column. Chemotactic bacteria experience longer residence time when accumulating near the NAPL sources, which results in lower percent recovery than that of nonchemotactic bacteria in the effluent over the observation period. Our models can elucidate the extent to which chemotaxis may accelerate bioremediation and assess the efficiency of bacterial chemotaxis for in situ analysis.

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Pore Structure Characterization and Numerical Simulation of Electrical Conductivity for Tight Sandstone by Digital Rock Physics

Authors: Xuefeng Liu[1]; Hao Ni[1]; Jingxu Yan[1]; XiaoWei Zhang[1]

[1] *China University of Petroleum*

Corresponding Author: liuxf@upc.edu.cn

The digital rock consisted of only two phases, solid matrix and pore space, is insufficient to calculate bulk properties of tight sandstone and shale accurately due to bimodal pore size distribution and high abundance of clay type. In this work, we proposed a multi-scale information fusion method to construct multi-mineral digital rock and predict electrical conductivity accurately. Core plug samples of tight sandstone are first scanned by X-ray Micro Computed Tomography (CT) to obtain 3-D gray scale images, from which macro intergranular pores can be identified. Then, energy-dispersive SEM (EDS-SEM) is performed on one end of the samples to obtain a mineralogy mapping which will be used as mineral registration to correlate greyscale ranges of 3-D images with minerals. 3-D multi-mineral digital rocks are obtained by multi-threshold segmentation. The fine structure of each mineral phase is revealed by Nano CT and high-resolution SEM technique, from which the micro porosities associated with each mineral phase are obtained by segmentation algorithm. Finally, the effective conductivity of each mineral phase is calculated by Archie equation or Waxman-Smits model. Then the voxels in 3-D digital rock are defined as conductors with variable effective conductivity. The bulk electrical conductivity of the multi-mineral digital rock is predicted by the Finite Element Method (FEM). The contribution of fluid in multi-scale pore space and clay minerals to the bulk electrical properties are implicitly fused in the numerical simulation method without increasing computational cost. The contents of major mineral components of multi-mineral digital rocks agree well with those measured by X-Ray Diffraction (XRD). The simulated electrical conductivities of water saturated rocks are in good agreement with experimental results in laboratory. The requests in constructing digital rock to predict bulk properties accurately are provided by analyzing the effect of clay type and micro CT scanning resolution on calculated electrical conductivity. The multi-scale information fusion method is based on the 3-D images of core plug samples, which allows us to compare the estimated conductivities with measured results in lab quantitatively. The method is the basis to predict electrical resistivities of partial water saturated rock and can be further applied to calculate other effective properties of tight sandstone and shale.

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Benchmarking root and soil interaction models exemplified with CRootBox and Dumux

Authors: Andrea Schnepf[1]; Daniel Leitner[2]

Co-authors: Bernd Flemisch [3]; Harry Vereecken [1]; Jan Vanderborght [1]; Timo Koch [3]

[1] *Institute of Bio- and Geosciences Agrosphere (IBG-3), FZ Jülich*

[2] *Simwerk*

[3] *Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart*

Corresponding Author: daniel.leitner@simwerk.at

Complex models of root architecture and function can increase our fundamental understanding of crop growth and function, and therefore will improve agricultural management strategies as well as root trait selection in plant breeding.

However, the analysis of such models is difficult. The variety of modelling approaches describing various processes lead to disagreement between the models. This discrepancy emerges from different root architecture development as well as different definitions of sink terms describing water and solute uptake. In Schnepf et al. 2019 (preprint) various research groups developed a systematic framework for benchmarking individual components of any root functional models. These components are root architecture, water flow and solute transport in soil and roots. For water movement and solute transport numerical aspects are of main interest, but also modelling aspects like the description of sink terms are analysed. Root architecture development is compared at a conceptual level as different models do not have a common process representation. Therefore, modelling results are compared to experimentally observed reference root systems.

Splitting root functional models into simpler sub components enables precise testing, quantitative inter-model comparisons as well as analysis of single common processes. We demonstrate the different benchmarks by applying them to the root growth model CRootBox (Schnepf et al. 2018) for root architectural development and DuMux (Flemisch et al. 2011) as porous medium solver for water flow and solute transport in both soil and roots.

We encourage other plant functional modellers to join this benchmarking effort. Therefore, the benchmark scenarios are presented in Jupyter Notebooks for easy accessibility and transparency (https://github.com/RSA-benchmarks/collaborative-comparison). Results of root architectural benchmarks will help interpret differences found in water and solute transport and uptake. Therefore, benchmarking will lead to greater confidence, avoiding that future work is based on accidental results caused by bugs, numerical errors or conceptual misunderstandings and will set a standard for model development.

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Research on Capillary Dynamic Effect during Water Displacement in Low Permeability Reservoirs

Authors: Aifen Li[1]; Zili Li[1]

[1] *Research Centre of Multiphase Flow in Porous Media , China University of Petroleum (East China)*

Corresponding Author: 1103123733@qq.com

The oil-water transition zone can be huge in low permeabile reservoirs with edge and bottom water. Because of the particularly small pore throat and the low permeability, the capillary pressure is one

of the important factors affecting the mechanism of water flooding. The traditional development theory uses the capillary pressure at the equilibrium of the oil-water interface, and does not consider the relevant factors such as displacement speed and rock wettability, resulting in large differences in numerical simulation and development dynamic prediction of low-permeability reservoirs. Well defined experiments and theoretically analyses are conducted to determine the importance of dynamic effect in capillary pressure relationships for two-phase flow in porous media. In this paper, A series of waterfloods have been performed at different flow rates. A self-developed dynamic capillary pressure test system was used to test the water saturation and oil-water two-phase pressure at different positions at different times in the water flooding process. Calculate the capillary dynamic coefficient τ, which is used to characterize the dynamic capillary pressure and study the mechanism of it. The research shows that with the increase of flooding speed, the viscous resistance in the displacement process gradually dominates, the more obvious the capillary dynamic effect, and the greater the water wetness of the rock, the larger the capillary pressure dynamic coefficient. It is of great significance to study the mechanism and law of capillary pressure curve changing with water flooding speed for further understanding of seepage law and prediction of development dynamics.
Keywords: Low permeability reservoir; water flooding; dynamic capillary pressure; capillary dynamic coefficient

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Determination of organic and inorganic saturations and permeabilities of shale gas reservoir

Author: YAJUN LI[1]

Co-authors: QIAN SANG [1]; MINGZHE DONG [2]

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

[2] *University of Calgary*

Corresponding Authors: mtdong@ucalgary.ca, sangqian163@163.com, liyajun@upc.edu.cn

Shale gas formations are complex and heterogeneous systems with both organic and inorganic contents. Shale gas is stored in porous reservoirs in three forms: free gas in the inorganic matrix pores and natural fractures, free gas in the kerogen pores, adsorbed gas on the surfaces of pores within organic matter. Consequently, total porosity of shale gas formation is composed of inorganic porosity and organic porosity, while total gas saturation is composed of inorganic gas saturation, organic gas saturation; furthermore, organic gas saturation consists of organic free-gas saturation and organic adsorbed-gas saturation. Identifying the relative proportions and permeabilities of gas stored in the three different forms is important to the accurate determination of the shale gas-in-place and the design of effective production strategies. Many studies have been performed to determine the production characteristics of the free gas and the adsorbed gas for shale gas reservoirs. However, limited research has been conducted on the storage features and mechanisms of variable gas forms, there is no reported research that identifies the organic and inorganic porosities, saturations and permeabilities of shale gas reservoirs. We therefore recently performed three types of vacuum-imbibition tests - water, methane and helium imbibition - on 26 shale gas rock samples to distinguish these petrophysical parameters. In case of 100% saturated experiments, the final imbibed methane volume represents the total methane content that a shale sample can hold, the final imbibed helium volume in helium imbibition test represents the total porosity, the final imbibed water volume in water imbibition test represents the inorganic content, and the difference between methane and helium imbibed volume represents the adsorbed methane content, the difference between water and helium imbibed volume represents the organic free-gas content. Thereby organic and inorganic porosities and saturations are obtained using the vacuum-imbibition method. Then, a mathematical model considering gas flow and adsorption by reference to well testing model was proposed to match the lab-measured imbibed volume - time curve. The inorganic/organic permeabilities for these shale samples were successfully determined using this approach. Experimental results indicate that, for

the shale rock samples tested, the organic porosity ranges from 23% to 43% of the total porosity, 31% averagely. 17% to 50% of the methane gas in place is adsorbed gas, 33% averagely. Methane gas in kerogen, containing organic free gas and adsorbed gas, ranges from 39% to 68%, 54% averagely. Both the organic saturation and the organic porosity exhibit a growing trend with total organic carbon of shale rock samples. The organic permeabilities of the samples used in this study were two or three orders of magnitude lower than inorganic permeabilities. The proposed methodology should be applied in shale gas resource evaluation and reservoir characterizations.

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Pore scale disorder on tensile fracturing of porous medium using Lattice method simulation

Author: WenXiang Tian[1]

Co-authors: Gang Ma [1]; Wei Zhou [1]; Yao Liu [1]; Lingxiao Chen [1]

[1] *Wuhan University*

Corresponding Authors: 2015301580042@whu.edu.cn, tian_wenxiang@whu.edu.cn, liuyao1996@whu.edu.cn, magang630@whu.edu.cn, zw_mxx@whu.edu.cn

It has been found that not only the porosity, but also the pore structure can influence the connectivity, permeability, stress-bearing capability of porous materials. In this study, we study the spatial pore distribution, and its effects on the mechanical behaviors such as the tensile fracturing of brittle porous medium. We generate a series of mesoscopic porous systems with different pore scale disorder. The pore disorder is quantified using Minkowski tensor. We then perform uniaxial tensile simulations using Lattice model, which is simple yet versatile and robust. By means of large scale and extensive lattice simulations, we investigate the relation between brittle fracturing and porosity, pore configuration of the model systems. The simulation results show that, there is a strong relation between the porosity, pore structure disorder, and mechanical behaviors. With the increase of porosity, the range of pore structure disorder decreases and the macroscopic tensile strength decrease. The cracks distributes randomly without forming a macroscopic percolation crack.

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Effect of Salinity on Water-Alternating-Gas (WAG) Injection in Microporous Media

Authors: Vishnu Bhadran[1]; Yit-Fatt Yap[None]; Afshin Goharzadeh[1]

[1] *Khalifa University*

Corresponding Authors: yap.fatt@ku.ac.ae, afshin_goharzadeh@yahoo.com, vishnu.bhadran@ku.ac.ae

Water-alternating-gas (WAG) injection in oil reservoirs is an enhanced recovery process. The main objective is to recover remaining oil in mature reservoirs by a use of alternate injection of water and gas into the reservoir with a given time period. WAG process contributes to a better sweep efficiency and can reduce gas channelling from injector to producer. This work is focused on experimental investigation of WAG injection in micro-porous media initially saturated with oil. Effect of salinity on residual oil saturation inside the micro-porous media is studied during WAG injection. The experimental setup consists of a transparent micro-channel of area 50 x 20 mm2, packed with glass beads of diameter 1.6mm, a dual-drive syringe pump having two glass syringes, a collection tank and a digital microscope for flow visualization. The horizontal micro-channel has a depth of 1.7 mm. In this study, brine solutions of various salinity (0<C<50K ppm) are prepared using vortex generator and are used to study the effects of salinity in WAG process in comparison with the deionized water. The image acquisition system consists of a microscope and a digital camera system to capture the real time image. Full-frame images of 1815×1151 pixels are acquired. The flow in the porous media is observed with a field of view 30 × 20 mm2. Image processing using Matlab codes are used to measure the remaining oil ganglia inside the micro-porous media after three cycles of WAG process. It was noted that for low saline concentrations (0<C<1000 ppm) the effect of salinity on first water flood is negligible. Whereas, for moderately and high saline water (with a concentration higher than 10,000 ppm) a significant impact on the amount of saturated oil present in the porous media is observed. It was noted that 65% of the residual crude oil was recovered after the first water flood with a saline concentration of 10,000ppm compared to 35% oil recovery achieved from the low saline brine samples. A significant increase in oil recovery was observed after each gas cycles with increasing water salinity due to less water saturation and less oil disruption. The recovered residual crude oil after three cycles of WAG process increases with the increase of salinity concentration in brine. These results might be linked to the viscosity of brine which becomes more viscous at higher salinity. Obtained experimental results can be used to understand the role of salinity in WAG processes, and can help to validate further numerical model related to this topic.

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Buoyancy-induced flow and heat transfer through and around a porous cylinder in a cavity

Authors: Shimin Yu[1]; Tingting Tang[2]; Jianhui Li[2]; Peng Yu[2]

[1] *Harbin Institute of Technology & Southern University of Science and Technology*

[2] *Southern University of Science and Technology*

Corresponding Authors: yup6@sustech.edu.cn, 11849524@mail.sustech.edu.cn, lijh@sustech.edu.cn, tangtt@sustech.edu.cn

Many engineering applications involve natural convection in porous media, such as electronic cooling, drying process, metal melting and solidification. Such phenomena of buoyancy-induced flow and heat transfer through and around a porous configuration include various fundamental mechanisms 1. In the present study, a two-dimensional numerical investigation is performed for steady natural convection from a porous cylinder with internal heat generation in a square cavity. Considering the Boussinesq approximation, the Navier-Stokes equation is used to model the flow in the clear fluid region, and the Darcy-Brinkman-Forchheimer extended model is applied for the porous medium region. For the interface between fluid and porous medium, the shear stress jump condition 2 and the continuities of velocity, normal stress, temperature, and heat flux are applied. Numerical simulations are carried out by applying the finite volume method based on the collocated body-fitted and multi-block grids. The flow and thermal characteristics in terms of streamlines, isotherms, and local and average Nusselt number will be investigated by considering the effects of the Darcy number (Da) and the Rayleigh number (Ra). The underlying physics will be discussed, which would provide useful guidance to improve the performance of related engineering applications.

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Mechanism of shale gas occurrence: Insights from comparative study on pore structures of marine and lacustrine shales

Authors: Lei Chen[1]; Keyu Liu[1]

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

Corresponding Author: chenlei19880804@163.com

The exploration practices of marine and lacustrine shale gas in the Upper Yangtze Platform, South China show that there is a huge difference in gas content, which is mainly related to the difference of pore structure. This study is focused on marine Longmaxi and lacustrine Da'anzhai shales in the Upper Yangtze Platform, and their pore structure characteristics were compared and the mechanism of shale gas occurrence were discussed. First, the pore structures of marine and lacustrine shales were characterized and the effects of organic matter abundance, maturity and inorganic minerals on porosity were investigated. Then the contributions of different components to porosity were evaluated and the occurrence mode of methane in the pores of marine and lacustrine shales was established. The results show that (1) Three pore types can be observed in both marine and lacustrine shales: organic matter-hosted pores (OM pores), framework minerals-associated pores (FM pores), and clay minerals-associated pores (CM pores). OM pores are more developed in marine shale and CM pores are more
developed in lacustrine shale. (2) Low pressure gas adsorption (LPGA) results show that the micropores of marine shale are dominated by pores of 0.4–0.7 nm and the micropores of lacustrine shale are dominated by pores of 0.5–0.9 nm, while the mesopores of marine shale are dominated by pores of 2–10 nm and the mesopores
of lacustrine shale are dominated by pores of 3–30 nm, which are consistent with MIP results. (3) Organic matter has an impact on porosity of marine and continental shales but is not the most important controlling factor. And
the contribution of organic matter to porosity in marine shale is greater than the contribution of organic matter to porosity in lacustrine shale. Shale porosity increases first and then decreases with the increase of maturity,
which may be related to the carbonization of organic matter. (4) OM pores and CM pores tend to be preserved due to the presence of rigid grains that form rigid frameworks preventing these pores from collapsing. FM pores are mainly related to the dissolution of framework minerals by organic acids, and these dissolution pores can greatly improve the porosity and permeability of shale. (5) Quantification of porosity as related to mineralogy shows that OM pores contribute approximately 37% to total porosity of marine shale and 24% to total porosity of lacustrine shale and CM pores contribute approximately 53% to total porosity of marine shale and 67% to total porosity of lacustrine shale. (6) Shale gas occurrence is mainly controlled by the distribution mode of pore systems which are composed of OM pores, FM pores and CM pores. It is due to higher percentage on OM pores and lower percentage on CM pores that gas content of marine shale is generally higher than that of lacustrine shale.

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Pore scale simulations of two-phase flow in porous media with high permeability

Authors: Maxime Cochennec[1]; Hossein Davarzani[2]; Yohan Davit[3]; Stéfan Colombano[2]; Ioannis Ignatiadis[2]; Michel Quintard[4]

[1] *BRGM (French geological survey) ; Institut de Mécanique des Fluides de Toulouse*

[2] *BRGM (French geological survey)*

[3] *Institut de Mécanique des Fluides de Toulouse*

[4] *Université de Toulouse, INPT, UPS, IMFT (Institut de Mécanique des Fluides de Toulouse), Allée Camille Soula, F-31400 Toulouse, France - CNRS, IMFT: F-31400 Toulouse, France*

Corresponding Authors: i.ignatiadis@brgm.fr, m.cochennec@brgm.fr, h.davarzani@brgm.fr, yohan.davit@imft.fr, s.colombano@brgm.fr

Two-phase flows in highly permeable porous media are encountered in a variety of applications, including trickle-bed reactors in chemical engineering (Attou et al. 1999), debris bed associated with accidents in nuclear safety (Clavier et al. 2017) or gravels in soil remediation. The physics of such flows is fundamentally different from that of most other porous structures, such as soils or rocks, where capillary effects are dominant. When the size of the pores is sufficiently large, the flow may be dominated by gravitational, inertial or viscous effects and standard Darcy-type models of two-phase flow in porous media may fail to accurately capture the flow.

Here, we ask whether generalized Darcy equations are adapted to describing two-phase flows in highly permeable structures, focusing on the expression of the capillary pressure and on coupling terms in the momentum transport equation (Rothman 1990, Li et al. 2005, Yiotis et al. 2007, Shams et al. 2018). We study a model system consisting of an array of cylinders in a thin square cuboid, resembling a Hele-Shaw flow-cell with obstacles. The flow is described by Stokes equations (creeping flow) for each phase integrated over the height (z-direction) of the cuboid. The radius of curvature of the interface in the z-direction is assumed to be of the same order of magnitude as the height of the system and the linear drag induced by upper/lower solid surfaces is estimated based on a Poiseuille profile in the z-direction.

The idea of using this model system is that, by changing the height of the cuboid, we can vary the permeability by orders of magnitude while leaving the rest of the geometry unchanged. This allows us to characterize the impact of the permeability while leaving the rest of the structural features identical. To do so, we solve the flow equations using the Level Set method and a finite element discretization. The code is validated by comparison with a Boundary Element Method, which relies on a surface discretization of the interface and a pseudo-analytical formulation in the bulk of the phases. This allows us to precisely locate the interface, even in the case of very thin film flow, and to carefully analyze the choice of parameters in the Finite Element formulation.

We find that the Level Set method allows us to capture accurately the position of the sharp interface and that results are particularly sensitive to the reinitialization parameter in the Level Set formulation. We observe a change in the topology of the non-wetting phase depending on the values of the capillary number and the ratio of fluid filtration velocities. This allows us to construct a map of the observed regimes and study the evolution of capillary pressure compared to standard representations. We also calculate the drag between the two fluid phases and compare it to the different components of the fluid/solid drags to assess the validity of generalized Darcy's laws and the need for coupling terms in the momentum transport equations.

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Poroelastic effects of CO2 adsorption capacity in coal seams under subsurface boundary conditions

Author: Yuxun Zhu[1]

Co-authors: Jinfeng Liu [2]; Peter Fokker [3]

[1] *School of Earth Sciences and Engineering, Sun Yat-Sen University, 510275, Guangzhou, China*

[2] *Sun Yat-Sen University, 510275, Guangzhou, China*

[3] *Department of Earth Sciences, Faculty of Geosciences, Utrecht University, 3584CD Utrecht, The Netherlands*

Corresponding Authors: peter.fokker@tno.nl, zhuyx27@mail2.sysu.edu.cn, liujinf5@mail.sysu.edu.cn

Coal seam is generally treated as an organic-rich, porous rock which contains coal matrix (solid) cut by a complex network of cleats and fractures (Laubach et al. 1998). Coal matrix has a large potential for CO2 adsorption and therefore deep, unmined coal seams have been considered as a potential site for CO2 geological storage in the context of carbon capture, utilization and storage (CCUS) strategies for mitigating global warming. However, CO2 adsorption, at equilibrium, makes coal matrix expand several percent, thus leading to changes in stress states of coal under in-situ subsurface boundary conditions (i.e. near zero lateral displacement boundary condition). More importantly, thermodynamic models and experiments have dominated that applied stress reduces CO2 adsorption capacity of coal matrix by 5-50% (Hol et al. 2011). This strongly suggests poroelastic effects of coal seams will have a significant influence on maximum storage capacity of CO2 that was usually estimated using the classical Langmuir model that omits the effect of applied stress on adsorption capacity. In this contribution, we attempt to determine the effect of poroelastic behavior of coal on (maximum) CO2 adsorption capacity that can be reached at equilibrium, by incorporating a fully coupled stress-strain-sorption model developed by Hol et al. (2012) and Liu et al. (2016) into a linear poroelastic model. Using the constructed model and proper parameter values, we calculated the maximum CO2 adsorption concentration of coal seams against the burial depth, for the first place. In the model, we considered the in-situ subsurface boundary conditions may lie in between such two end-member boundary conditions, i.e. constant stress boundary condition which allows coal to expand freely, and zero lateral displacement boundary conditions which allows coal to expand in vertical direction only. The model results demonstrate that the maximum concentration of CO2 adsorbed for a certain coal rank estimated using our constructed model under zero-displacement boundary conditions yield ~0.54 mmol/gcoal at a depth of ~820 m, while the results predicted by Langmuir model increase with the burial depth, at given stress-pressure-temperature conditions. We also analyzed the sensitivity of the adsorption concentration to Biot's coefficient (α) and found that the adsorption concentration of CO2 in coal seams systematically increased with the Biot's coefficient. The largest difference in adsorption concentration was ~0.27 mmol/gcoal between α=0.2 and α=0.8, reflecting a crucial influence of the cleat system in coal seams on CO2 adsorption capacity. Furthermore, we applied our constructed poroelastic model to estimating maximum CO2 adsorption capacity in a coal seam surrounded by dense sandstone with high stiffness, which is located in Shizhuang Block of Qinshui Basin at a burial depth of 626 m. The model results indicated the maximum adsorption capacity of ~0.72 ton/m2, suggesting that Shizhuang block has a potential used for carbon geological storage. Note that our model now focused on equilibrium state only, and the full coupled stress-strain-sorption-diffusion-permeability process will be considered in the on-going research.

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Properties Quantification of Heterogeneous Media with 3D Vision informed Machine Learning

Author: Omar Al-Farisi[1]

Co-authors: Aikifa Raza [2]; Hongtao Zhang [3]; Djamel Ouzzane [4]; Mohamed Sassi [1]; Tiejun Zhang [2]

[1] *Khalifa University of Science and Technology*

[2] *Department of Mechanical Engineering, Masdar Institute, Khalifa University of Science and Technology, P.O. Box 54224, Abu Dhabi, UAE.*

[3] *Department of Mechanical Engineering, Masdar Institute, Khalifa University of Science and Technology, P.O. Box 54224, Abu Dhabi, UAE*

[4] *Abu Dhabi National Oil Company*

Corresponding Authors: aikifa.raza@ku.ac.ae, alfarisi@live.ca, djouzzane@adnoc.ae, hongtao.zhang@ku.ac.ae, mohamed.sassi@ku.ac.ae, tiejun.zhang@ku.ac.ae

Flow simulation models of heterogeneous porous media use rock types and their properties for predicting future fluid behavior. Rock type represents a unique set of static and dynamic properties. Mineralogy, capillary pressure, and permeability are some of the static properties. Relative permeability and wettability are some of the dynamic properties. Scientists uneasily researched to quantify these properties from Micro-Computed-Tomography (uCT) or Magnetic Resonance Imaging (MRI) vision, either based on Image Processing or combined Image Processing with Machine Learning (IPML). Each approach has its strengths and weaknesses, as identified in the literature and our demonstration with experimental reference calibrators. One of the challenges faced the scientists is the inability of 2D images to capture heterogeneity. Another challenge is properties determination from a 3D vision of the homogenous porous system appeared non-usable for the heterogeneous media. Through designing and uCT/MRI imaging of multiple 3D micromodel references, we propose an appropriate path to quantify properties of heterogeneous porous media. When Image Processing delivers with high accuracy the porosity, identifying other properties like mineralogy and permeability, IPML provides better prediction, but at the expense of computer power and processing time. A trade-off between accuracy and time is critical in machine learning aided analysis of heterogeneous porous media for efficient properties determination.

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Unsteady mixed convection flow through and around an array of cylinders

Author: Tingting Tang[1]

Co-authors: Shimin Yu [2]; Jianhui Li [1]; Peng Yu [1]

[1] *Southern University of Science and Technology*

[2] *Harbin Institute of Technology&Southern University of Science and Technology*

Corresponding Authors: yup6@sustech.edu.cn, 11849524@mail.sustech.edu.cn, tangtt@sustech.edu.cn, lijh@sustech.edu.cn

Mixed convection flow through and around an array of cylinders is of great significance for various engineering applications such as micro heat exchangers, cooling electronics, and fuel cells. The array of cylinders was usually treated as a permeable body in the previous studies [1, 2]. In the current work, we directly simulate the flow through and around an array of multiple cylinders under the

effect of thermal buoyancy. The opposing buoyancy was found to have significant effect on the vortex shedding behind a single heated cylinder 3. Also, studies on opposing buoyancy appear far less than those on aiding buoyancy. Therefore, the present study is focused on the influence of opposing buoyancy on the wake behavior behind an array of cylinders.

We will present a two-dimensional numerical study for unbounded mixed convection flow through and around a square array of 10 10 circular cylinders. The Reynolds number is 100 for typical unsteady laminar flow and the Prandtl number is 7 for water. The effects of the geometry and the thermal buoyancy on the flow and heat transfer characteristics will be investigated by varying the solid fraction of the array and the Richardson number. The governing equations will be solved by using finite-volume method with body-fitted mesh and the numerical scheme will be validated against standard cases of flow around a single heated cylinder. The complex flow and heat transfer features will be presented in the form of mean and instantaneous velocity, vorticity, streamlines, and temperature distributions. The global parameters of drag and lift coefficients, Strouhal number, and Nusselt number will be investigated. Moreover, the effects of inertial force within the array and the connection between local and global characteristics will be discussed.

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Capillary Pressure of Non-Wetting Ganglia in Porous Media: a Sub-Darcy Model

Authors: Chuanxi Wang[1]; ke xu[None]

[1] *13880070771*

Corresponding Authors: xukethu@mit.edu, 2001111738@pku.edu.cn

Capillary pressure (*Pc*) of dispersed ganglia (bubbles, oil droplets, carbon dioxide clusters etc.) in porous media plays dominant role in residual fluid mobilization, ripening, dissolution and growth, therefore is essential in description of hydrocarbon recovery, carbon dioxide geological sequestration, and water management in fuel cell. However, the size of a residual fluid ganglion is limited in finite number of pores, which invalidates the Darcy-scale description of *Pc* as a function of saturation, wettability, and size distribution. Therefore, a sub-Darcy scale description of *Pc* for residual ganglia is required [Xu, et al., *PRL*, 2017; de Chalendar, et al., *JFM*, 2018; Lin, et al., *WRR*, 2017].

We propose a conceptual pore-scale model [Fig.1(a)] for *Pc* of a non-wetting ganglion statically trapped in an ideal two-dimensional porous medium. The porous medium consists of regularly arranged identical grains[Fig.1(b)]. We rigorously derive the relationship between ganglia volume (V) and *Pc*, and study how geometric parameters (grain size, pore-throat ratio, pore occupancy) and history (growth, shrinkage, coalescence) modify *Pc* - V correlation.

Surprisingly, the *Pc* - V relationship in pore-scale is non-monotonic and non-continuous [Fig.1(c)], qualitatively distinct from Darcy-scale description. With V increasing, a ganglion experiences three stages: (1) when the ganglion is too small to be confined by pore geometry, it behaves like a free

bubble and *Pc* decreases; (2) when the ganglion is large enough that the converging pore-throat geometry deforms it, *Pc* starts to increase with *V* ; (3) after fulfilling the space of occupied pores, it invades into a neighboring pore, and an abrupt re-distribution event (burst) may happen to approach local equilibrium which leads to an sharp decrease of *Pc*. When the ganglion further grows, the above recycle repeats, resulting in fluctuating and non-continuous of *Pc* - *V* curve.

We observe pore-scale hysteresis effect: a growing ganglion and a shrinking ganglion have different curves [Fig.1(c)]. In addition, a ganglion of a given *V* has multiple stable status (corresponding to multiple pore occupancy), and it is at global surface energy minimum when it is at an intermediate, rather than the maximum or minimum, pore occupancy. This multistability is one of the origins of hysteresis in Darcy scale media. This finding agrees with the mesoscale conceptual model proposed by Cueto-Felgueroso and Juanes [*GRL*, 2015].

When the pore occupancy of a ganglion goes to infinite, the *Pc* - *V* curve merges with the Darcy scale description in a homogeneous porous medium [Fig.1(c)]. That said, when the ganglia is growing (drainage), *Pc* approximates to the entry pressure at the throat; when a ganglion is shrinking (imbibition), the *Pc* approximates to the minimum possible capillary pressure in the system.

We believe that this work opens a door for more accurate and more physically-solid modeling of bubble and droplet trapping-mobilization in porous media.

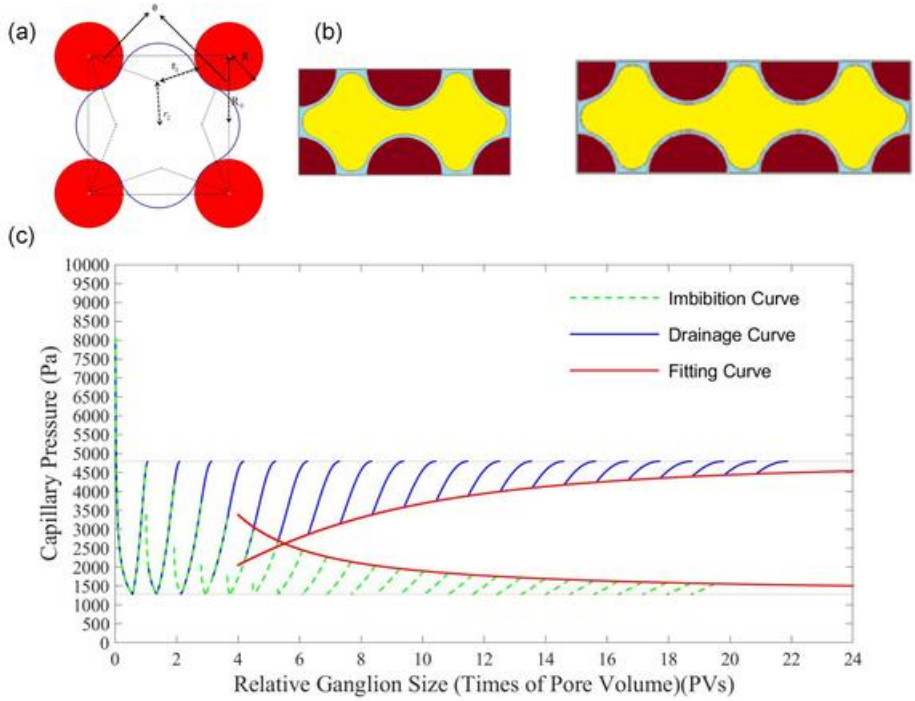

Figure 5: (a) A conceptual pore-scale model for Pc of a non-wetting ganglion. (b) Ganglion of different pore occupancy. (c) The non-monotonic and non-continuous Pc - V relationship.

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Turbulent mixing in the hyporheic zone

Author: Elisa Baioni[1]

Co-authors: Giovanni Porta [2]; Mohaddeseh Mousavi Nezhad ; Alberto Guadagnini [2]

[1] *University of Warwick*

[2] *Politecnico di Milano*

Corresponding Authors: alberto.guadagnini@polimi.it, giovanni.porta@polimi.it, m.mousavi-nezhad@warwick.ac.uk, e.baioni@warwick.ac.uk

Predictive modeling of turbulent mixing in the Benthic Biolayer of rivers is key to develop sustainable and cost-effective strategies for surface water purification mediated by biomass present in the sediment bed. These aspects are typically addressed through numerical models which are developed on the basis of computational fluid dynamics approaches to simulate turbulent flow in porous media (Kuwahara et al., 1998) and are then coupled to solute mixing models. The latter attempt to simulate turbulent mixing in porous sediments, an advection-dispersion approach being employed to simulate the exchange of solutes between surface water and groundwater (Lautz and Siegel, 2006). Most of the available modeling approaches rest on the assumption that the diffusion coefficient can be considered as constant across the sediment depth, which is not entirely consistent with interpretations of documented laboratory investigations (Chandler et al., 2016).
It is recognized that mixing in such a critical region can be influenced by turbulence and some studies attempt to assess the dependency of the diffusion coefficient on macroscopic characteristics of flow (Nagaoka and Ohgaki,1990). In this context, we have recently assessed the capability of classical models employed to characterize mixing in the hyporheic zone upon relying on a stochastic inverse modeling approach conditional to experimental observations. While our approach yields depth-resolved posterior probability distributions of the diffusion coefficient, it is noted that the reliability of the above mentioned models to depict mixing is considerably reduced in the region where fluid show an enhanced and complex turbulent behavior (i.e., in the vicinity of the water-bed interface). This is partly due to the observation that temporal fluctuations of velocity taking place at the pore scale can critically affect the macro-scale system behavior and should be included in effective mixing models.
Our work aims at investigating solute transport and mixing in a porous medium under turbulent flow conditions. The study is grounded on the use of the random walk technique and an appropriate Lagrangian mixing model. The former is employed to track the motion of solute particles due to diffusion processes (Leyay, 2012), the latter enabling evaluation of the temporal evolution of chemical concentration in the hyporheic zone, as well as mixing of the solute mass within the porous domain. Results are then compared against experimental data quantifying the variation of the effective dispersion coefficient with depth below the sediment-water interface (Chandler et al., 2016).

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Gravity-driven fluid slug splitting at T-junctions: visual experiments and a novel model

Authors: Zhibing Yang[1]; Song Xue[1]; Yi-Feng Chen[1]

[1] *Wuhan University*

Corresponding Authors: csyfchen@whu.edu.cn, songxue@whu.edu.cn, zbyang@whu.edu.cn

A fundamental understanding of fluid slug flow behavior in a network of microchannels is of critical importance both scientifically and technologically. Here, we present an experimental and modeling study of the gravity-driven water slug flow behavior at T-shaped intersections. In the experiments, the flow processes are visualized, and the flow dynamics are quantitatively analyzed. We develop a fast, novel computational model that adequately captures the flow dynamics. Using the Voinov—Box law to calculate the dynamic contact angles, this model solves temporal evolution of interface motion based on force balance with the quasi-static assumption at each time step. By both experiments and simulations, we carefully examine the influence of various physical parameters on the flow splitting behavior, including the widths and inclination angles of channels, slug lengths, and dynamic contact angles. We elucidate the mechanisms behind the intricate balance between gravitational, capillary, and viscous forces that controls the flow splitting regimes.

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Governing equations of orthogonal nonlinear flow in porous media

Author: Chengwei QI[1]

[1] *Chongqing University of Science and Technology*

Corresponding Author: field_theory@163.com

Using vector field theory, the governing equation of orthogonal high-velocity nonlinear flow in porous media is obtained for the first time by expanding and simplifying the velocity-free equation, which is derived by substituting the explicit function from pressure gradient to macroscopic velocity of fluid flowing in porous media solved from Forchheimer equation into the continuity equation of fluid flowing in porous media. The governing equation of orthogonal high-velocity nonlinear flow in porous media and the governing equation of orthogonal low-velocity nonlinear flow in porous media will be collectively referred to as the governing equations of orthogonal nonlinear flow in porous media. While the symbolic solutions are out of reach because the governing equations of orthogonal nonlinear flow in porous media are rather cumbersome, the flow field geometry of orthogonal nonlinear flow in porous media is analyzed by using vector field theory and differential

geometry knowledge. Then a correct understanding is demonstrated that the conformal mapping cannot be used for analyzing orthogonal nonlinear flow field in porous media other than fields in which all streamlines are always straight. In order to bypass the boundary conditions in solving the governing equation of orthogonal nonlinear flow in porous media for symbolic solutions, applying the complex potential function and the metric tensor function from the "general kinematic formula for steady flow velocity field", the governing equation of orthogonal nonlinear flow in porous media in the Cartesian coordinate system is transformed into governing equation of orthogonal nonlinear flow in porous media in the corresponding potential-stream coordinate system for a given problem. In view of the fact that the governing equations of orthogonal nonlinear flow in porous media in the potential-stream coordinate system are still cumbersome, that is, the symbolic solutions for variable-directions flow field are difficult to obtain directly, it is suggested to search possible mapping that can indirectly obtain the symbolic field functions of orthogonal nonlinear flow in porous media.

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A new method for calculating displacement pressure based on total porosity of rock

Author: Runsen QIN[1]

Co-authors: Long Cao ; Ming YANG [2]; yuang Lei ; Yang Li

[1] *Research Institute of Tianjin Branch, CNOOC Energy Technology& Services Co.*

[2] *Tianjin Branch of CNOOC (China) Co., Ltd*

Corresponding Authors: leiyuan@cnooc.com.cn, yangming18@cnooc.com.cn, liyang51@cnooc.com.cn, caolong2@cnooc.com.cn, qinrs@cnooc.com.cn

Displacement pressure is an important parameter for reservoir evaluation, which is related to rock pore structure and mud content. Displacement pressure is obtained by experimental methods, and data are often limited due to the high cost of coring and test, which cannot fully meet the needs of oilfield exploration and development. Therefore, it is often necessary to establish a calculation model to get displacement pressure at different depths and different lithologies. Based on 89 samples analysis in BZ34 area,the correlation between displacement pressure and total porosity of samples is regressed. At the same time, the compaction model of siltstone and mudstone can be obtained by logging data respectively. The volume model is used to determine the total porosity of the mixed rock so as to obtain the displacement pressure values under different lithology and depth conditions. The results show that mud content is an important factor in establishing the relationship between displacement pressure and total porosity of samples, and the correlation coefficients between different mud contents reach up to 0.7. The total porosity by volume model can be simulated with an accuracy up to 80%. It is cost-effective that displacement pressure of rock at different depths and different lithology can be calculated by total porosity of the rock.

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Thermal stimulation to activate the desorption of shale gas over organic-rich shales

Authors: Xinlei Li[1]; Lijun You[1]; Yili Kang [1]; Jiang Liu [1]; Mingjun Chen[1]

[1] *State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu 610500, China*

Corresponding Authors: wendao92@qq.com, chenmj1026@163.com, 1663642144@qq.com, cwct_fdc@163.com, youlj0379@126.com

Shale gas production plays an important role in natural gas supply. Horizontal drilling and multi-stage hydraulic fracturing are the two key enabling technologies for the economic development of shale gas reservoirs. It is generally accepted that shale gas is mainly comprised of free gas in natural fractures and intergranular porosity and gas absorbed onto kerogen and clay-particle surfaces whose content is about 20%~80%. The initial decline in shale gas production is rapid, and the late production decline is slow, mainly due to the desorption of shale gas. The degree of shale gas desorption directly affects the production of shale gas wells.

Thermal stimulation, which is presented as formation heat treatment to remove formation damage such as pore-throat constriction and water-trapping damage caused by drilling, completion or hydraulic fracturing. In recent years, this technique is regarded as a new method to enhance shale gas recovery.

In this paper, the organic-rich shale of Longmaxi Formation is taken as the research object. A series of isothermal adsorption experiments of shale samples by fracturing fluid damage as well as before and after heat treatment from 400℃ to 600℃ are carried out. Based on the monolayer Langmuir isotherm, the impact of temperature on the isothermal adsorption/desorption characteristics of shale gas is investigated. The key factors that control the adsorption/desorption behavior of natural gas in shale formation mainly contain TOC (Total Organic Carbon), organic matter type, thermal maturity and clay minerals. We can transform the adsorption gas into free gas by pyrolyzing organic matter and Clay dehydration. The result shows that we can enhance shale gas recovery by altering the adsorption of kerogen and clay-particle surfaces through elevating formation temperature.

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Quantifying Wettability Alteration Effects on Fluid Flow Properties of Heterogeneous Porous Media

Author: Omar Al-Farisi[1]

Co-authors: Kamel Zahaf [2]; Djamel Ouzzane [3]; Mohamed Sassi [1]

[1] *Khalifa University of Science and Technology*

[2] *ADNOC Offshore*

[3] *Abu Dhabi National Oil Company*

Corresponding Authors: zahaf@adnoc.ae, alfarisi@live.ca, djouzzane@adnoc.ae, mohamed.sassi@ku.ac.ae

Scientists worked tremendously to address the effects of wettability alterations on fluid flow. Most of this work focused on two ways, flooding experiments and Simulation. Although tests deliver the wettability impact on multi-phase flow, specifically on relative permeability, they did not provide analytical reasoning. The simulation approach mainly runs the Lattice Boltzmann Model, which makes the results profoundly affected by the limitations of the assumption. Scientists and engineers need an efficient and robust path to quantify wettability from its physical and chemical properties. During our Research, in investigating the effect of wettability on fluid flow, we found that geometrical analysis has been a neglected factor. We observed the deformation of flow path geometry with the alteration of wettability. We start by determining the preferential wettability of porous media, then identifying the corresponding pore throat size for homogenous system or pore throat size morphology of the heterogeneous network. We assess the deformation of pore throat size due to wettability alteration using geometrical analysis. Then analytically produce relative permeability curves of the altered wettability porous system. Our research provides an analytical approach of quantifying wettability effects to create relative permeability with a simulation-free solution.

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The effect of tortuosity on relative permeability of porous media

Author: Fuyong Wang[1]

Co-authors: Liang Jiao [1]; Jiao Liang [1]

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

Corresponding Author: wangfuyong@cup.edu.cn

Relative permeability is significant for multi/two-phase flow in porous media. The classical relative permeability models, such as Purcell model (1949), Burdine model (1953), Corey model (1954), Brooks-Corey model (1966), assume that the tortuosity of pores with variable size is the same. The effect of variable tortuosity on relative permeability is not well studied. Based on the fractal characteristics of pore size distribution (PSD) and tortuosity in porous media, this paper presents a generalized analytical model of relative permeability in unsaturated porous media. The research results show that the relative permeability is the function of normalized wetting phase saturation, fractal dimension of PSD, fractal dimension of tortuosity, and the ratio of minimum pore radius to the maximum pore radius. The increasing PSD fractal dimension and tortuosity fractal dimension can significantly reduce wetting phase relative permeability, but the increase in nonwetting phase relative permeability is insignificant. Besides PSD fractal dimension and tortuosity fractal dimension, the ratio of minimum pore radius to the maximum pore radius affects the shape of relative permeability curves. With ratio of the ratio of minimum pore radius to the maximum pore radius decreases, the relative permeability of wetting phase can be reduced, but the change in nonwetting phase relative permeability is insignificant. Compared with the work presented by Li (2010), the novelty of the relative permeability model is the tortuosity fractal dimension was introduced in this paper. The assumption that every capillary tube has the same tortuous length in conventional relative permeability models

(Corey, 1954; Brooks and Corey, 1966; He and Hua, 1998; Li, 2008; Li, 2010) might be too ideal for the porous media with complex pore structures, such as tight sandstones/carbonates or shales, and tortuosity fractal dimension can provide another parameter to characterize complex pore structures besides PSD fractal dimension.

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Carbon Dioxide Sequestration of Fuel Combustion Exhaust Using Metal-Organic Frameworks (MOFs): A Molecular Simulation Study

Authors: Jie Li[1]; Jiaxiang Liu[1]; Wenquan Tao[1]; Zhuo Li[1]

[1] *State Key Laboratory of Pollution Control and Resource Reuse, International Joint Research Center for Sustainable Urban Water System*

Corresponding Authors: zhuoli2013@tongji.edu.cn, 1830566@tongji.edu.cn, iceliujiaxiang@tongji.edu.cn

As the most important anthropogenic greenhouse gas, CO₂, accounting for 70

The M-MOF-74 (M = Mg、Zn、Co、Ni, DOBDC⁴⁻ = 2,5 dioxido-1,4-benzenedicarboxylate) series has 1D hexagonal channels with a pore size of around 11-12Å, and contain a very high density of open metal sites [4]. Strong interaction between gas molecules and exposed metal cations makes M-MOF-74 especially suitable for storing various gases, such as H₂, methane, CO₂, and hydrocarbon separation. They have great application potential in carbon capture [5].

In this paper, the M-MOF-74 (M = Mg、Zn、Co、Ni) series is numerically investigated to separate and enrich CO₂ in the combustion exhaust of power plants and industrial factories. The components of exhaust are complex due to the presence of H₂O, SO₂ and other interruptions, thus the four materials are modified to improve its effectiveness. Based on the grand canonical Monte Carlo (GCMC) simulation and molecular dynamics (MD) simulation, the adsorption process of CO₂ molecules in materials is simulated, and the parameters are calculated, such as adsorption capacity, radial distribution function (RDF), adsorption heat, adsorption separation ratio, etc. The adsorption isotherms of Mg-MOF-74 show the highest adsorption capacity (360 mg/g at 0.15bar and 298 K) and the density distribution indicates that most of the CO₂ molecules are concentrated around the metal clusters.

The simulation results show good agreement with experimental data, and illustrate that Mg-MOF-74 is a promising candidate for CO₂ capture in combustion exhaust due to its high uptake capacity and favorable selectivity. The adsorption site and enthalpy of adsorption help us to explain the microscopic mechanism during the adsorption process. These works can provide theoretical guidance to unlock the actual gas adsorption mechanism for experimental fabrication of MOFs and CO₂ separation.

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Simulation of flow characteristics of nanoparticles in porous media using LBM

Authors: Chunyuan Gu[1]; Rongsheng Qin[None]

Co-author: Songlin Liu

[1] *13482354545*

Corresponding Authors: 1611225283@qq.com, wein1989@163.com

Nano-fluid drag reduction technology was developed for the problem of "high pressure but under-injection". The nano-fluid made with strong hydrophobic nanoparticles was injected into the target layers of the injection well. After stopping injection for a certain time, nanoparticles are adsorbed on the pore wall, which can significantly change the wettability of the reservoir, and then injection pressure greatly reduced. So It is of great significance to study the transporting and adsorbing of nanoparticles in pores for improving this technology.
The digital core of a low-permeability core from JS oil field is reconstructed by CT scanning carried out in Shanghai Synchrotron Radiation Facility (SSRF). The resolution is as high as 0.625 microns, and the average pore size is about 0.7 microns. By overlapping adjacent slices of the digital core, a two-dimensional core model is obtained, which is of good connectivity and has pores close to actual cores pores. Direct numerical simulations of the migration of nanoparticles in random generated digital cores and CT scan cores have been performed using Lattice Boltzmann method (LBM) coupled with discrete element method (DEM). A soft-sphere model was used to deal with particle-particle collisions and particle-wall collisions; the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory was used to calculate the non-contact force, taking into account the electrical properties of the particles and pore walls, the particle size , the strong adsorption between the particles and pore wall surface. besides, the effects of Brownian motion was also considered; the LBM is employed with an immersed moving boundary method for the fluid–structure interaction. A in-house OpenCL based Parallelized code was developed to deal with the massive calculation of direct numerical simulation.
The migration of 50nm diameter particles in core pores is studied. the simulation results show that nanoparticles can flow through in the larger channel smoothly, and they will collide with the pore wall at sharp bends by interception, and be captured and adsorbed by the pore wall; it is easy to form bridge plugs when aggregation of particles passing through a narrow pore throat; when the

flow velocity is large, it is not easy to form bridge plugs, and most of them will be washed out by the water flow.The results also show that factors such as salinity, and electrical properties of particles and pore wall, have significant effects on the migration of nanoparticles. High salinity makes nanoparticles tend to be agglomerative, which exacerbates blockages in the core. When the non-contact force between pore wall and particles are attractive, the amount of particles adsorbed on the pore wall would increase significantly. During the flow process, the main mechanism for particles capture in the core is straining , bridging and adsorption.

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The Impact of Pressure-Dependent Interfacial Tension and Contact Angle on Capillary Trapping and Storage of CO2 in Aquifers

Author: Bo Ren[1]

Co-authors: Ian Duncan [1]; Frank Male [1]

[1] *The University of Texas at Austin*

Corresponding Authors: frmale@utexas.edu, ian.duncan@beg.utexas.edu, boren@utexas.edu

CO2 capillary trapping increases the total amount of CO2 that can be effectively immobilized in saline aquifers. This trapping, manifesting itself as accumulated CO2 columns at a continuum scale, is due to threshold effects that occur below capillary barriers to flow. Considering that capillary pressure is dictated by pore throat size (which can be very heterogeneous), the trapped CO2 column height and associated CO2 saturation will vary spatially within a storage aquifer. This variation will be influenced by two pressure-dependent interfacial parameters: interfacial tension and contact angle. This statement epitomizes our objective here: to understand how the pressure-dependence of the two parameters affect the heterogeneity of capillary trapped CO2.

We consider the heterogeneity of capillary trapping using a real saline reservoir in the San Andres formation of the Permian Basin. The formation can be up to 2600 ft (around 800 m) thick (He et al., 2019). This large vertical extent is associated with a change in hydrostatic pressure of approximately 8 MPa between the shallow and deep part. Each carbonate micro-facies (dolomite mudstone, dolo-wackestone, dolo-packstone, and dolo-grainstone) are characterized by differing distributions of pore throat sizes.

Our conceptual model is a one-dimensional two-layer system with the upper layer being a flow barrier (low permeability) and the lower layer being a flow path (high permeability). The inputs to this model include microfacies-dependent capillary pressure versus saturation curves and permeability values. The capillary pressure curves were measured using the centrifuge technique, on the San Andres cores sampled from each microfacies. Then, we employed the Leverett j-function to scale the capillary pressure curve for the two layers in the context of each fabric. During scaling, we considered the influence of pressure on both the interfacial tension and contact angle of the CO2/brine/dolomite system, using the experimental measurements by Al-Yaseri et al. (2017) and Pereira et al. (2017). We varied the layer permeability contrast ratio from 5 to 20, based on our geology knowledge of San Andres formation. We also considered different combinations of microfacies that were assigned to the two layers with consistent permeability-capillary pressure relationships. Finally, through assuming capillary-gravity equilibrium (Lake et al., 2014)., we calculated the CO2 saturation buildup corresponding to different trapped CO2 column heights (i.e., 0, 0.05, 0.5 m). The CO2 saturation buildup is defined as the CO2 saturation in the lower layer minus that in the upper one.

We found that the saturation buildup can be up to 2X larger in the shallow part of the aquifer than in the deep one, after considering pressure-dependent interfacial tension and contact angles. Thus, assuming the two parameters to be constant across a storage aquifer with a large vertical extent would cause large errors in the quantification of capillary trapping of CO2 for field-scale flow simulations.

This study demonstrates the importance of considering pressure-dependent interfacial properties in predicting the vertical distribution of CO2. This has implications in developing a better understanding of leakage risks and consequent safety of storage.

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A multilevel quasi-Monte Carlo method for subsurface compressible single-phase flow with uncertainty in permeability

Authors: Yahong Xiang[1]; Xianbing Luo[1]

[1] *School of Mathematics and Statistics, Guizhou University, China*

Corresponding Authors: xbluo1@gzu.edu.cn, 497878069@qq.com

Permeability refers to the ability of rock to allow fluid to pass through under a certain pressure difference. It is not only related to porosity, but also to pore structure. Porosity and pore structure usually are uncertainty. Therefore, a stochastic method is useful to describe the influence by the uncertainty caused by permeability input on the output quantity of interest in the subsurface.

The Monte Carlo (MC) method is a common method for uncertainty quantification. The mean square error of MC is directly proportional to the estimation of variance and inversely proportional to the number of samples. To reduce the convergence error, the multilevel Quasi-Monte Carlo (MLQMC) method was used which combined the multilevel method with Quasi-Monte Carlo (QMC) sampling for the reduction of the variance estimator and modify the statistics separately.

In this paper, the multilevel method is based on finite element approximation of increasing accuracy sequence with decreasing space step sequence. MLQMC is to assess uncertain single-phase flow and transport within a lognormal random permeability field and compared with MLMC. It is found that QMC integration rules offer the prospect of a higher accuracy for the same computational cost compared to standard Monte Carlo integration, or a lower cost for the same accuracy. Interesting numerical examples will be provided.

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Stochastic apparent permeability model considering pore-throat structures and fluid-solid molecular interactions for shale oil reservoir

Authors: Jilong Xu[1]; Yuliang Su[1]; Wendong Wang[1]; Han Wang[1]

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

Corresponding Authors: wanghan.petro@gmail.com, jilongxu666@163.com, wwdong@upc.edu.cn, suyuliang@upc.edu.cn

Permeability is one of the most basic formation-rock properties needed to effectively develop shale reservoirs. Matrix permeability in many shale reservoirs can range from tens to hundreds of nanodarcies. The extremely low permeability of these formations can cause a large amount of time spent in measuring the apparent permeability (AP) by experiments. Even though numerous theoretical models incorporating the influence of pore size distribution and gas-slippage behavior on AP were proposed, few literatures have studied the impact of pore-throat structures and fluid-solid molecular interactions upon AP of shale oil reservoir.
In this work, we incorporate a more detailed description of pore-throat structures and fluid-solid molecular interactions to improve the apparent permeability analysis of strongly heterogeneous shale oil formations. A stochastic model is proposed by using SEM images, pore size distribution and PVT data of shale oil. Specifically, we first construct a spatial stochastic distribution model of organic matter and inorganic matrix, based on the patch size distribution of organic matter obtained from SEM images. Then, a certain pore size is allocated to each grid of spatial distribution model according to the pore size distribution in different media. To account for the variation of pore-throat radius, we introduced trigonometric functions and pore-throat ratio to represent the pore-throat structure parameters. The AP of shale oil in each grid is calculated by considering the different fluid-solid molecular interactions (represented as the difference of contact angle) and PVT parameters in the two media. Finally, we upscale the AP to the model scale through numerical simulation method. The results show that the additional resistance caused by throat structures will decrease the AP, and its influence degree is positively correlated with contact angle. With the increase of throat-pore ratio and contact angle in inorganic matrix, especially when the angle is more than 140 °, AP will increase significantly. However, the increase of contact angle in organic matter has little effect on AP. This is because the pore size in organic matter is an order of magnitude smaller than that of inorganic matrix. Therefore, when the TOC increases, the AP gradually decreases.
The stochastic model can well reflect the influence of pore-throat structures and fluid-solid molecular interactions on the AP of shale oil. Moreover, the model only needs a few minutes to determine AP, which is in good agreement with that obtained by experiments.

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Accelerated generalized multi-scale approximation of mixed finite elements method in subsurface porous media

Author: tao zhang[1]

Co-authors: Jie Chen [2]; Shuyu Sun [3]

[1] *King Abdullah University of Science and Technology*

[2] *Xi'an Jiaotong-Liverpool University*

[3] *King Abdullah University of Science and Technology (KAUST)*

Corresponding Authors: shuyu.sun@kaust.edu.sa, tao.zhang.1@kaust.edu.sa, jie.chen01@xjtlu.edu.cn

Multi-scale phenomena extensively exist in subsurface flows, while such multi-scale methodology can save much CPU time used for reservoir simulation and thereby enhance the capability of current reservoir simulators to be extensively applied in field-scale studies. Uncertainty qualification is a significant challenge hindering the development of multi-scale techniques due to the complex geometric distributions in subsurface rock structures. Permeability, the most cared properties in subsurface reservoirs, can span multiple scales and be of several orders of magnitude,and the thicknesses of these layers are much smaller than the domain size. Various boundary conditions and source terms are always needed to repeatedly solve the subsurface fluid flow problems. As a result, the model reduction technique that can reduce the degrees of freedom significantly is highly required by the reservoir simulation academy as well as the petroleum industry. In this work, a frame work of the mixed generalized multi-scale finite element method (GMsFEM) for solving Darcy's law in heterogeneous media will be studied, and pressure will be solved in multi-scale function space that is between fine-grid space and coarse-grid space while velocity is solved directly in the fine-grid space. A better accuracy can be obtained using this approach and the computational cost does not increase because of the good property of velocity matrix. Moreover, the proposed method preserves the local mass conservation property that is important for subsurface problems. Furthermore, we are using deep learning algorithms to accelerate the multi-scale approximations by constructing the multi-scale basis functions with the help of deep neural networks. Network hyperparameters are tuned and the structure is optimized to preserve the accuracy at the same time of improving efficiency.

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Physics-Preserving Algorithms for Flow and Transport in Porous Media

Author: Shuyu Sun[1]

Co-author: Huangxin Chen [2]

[1] *King Abdullah University of Science and Technology (KAUST)*

[2] *Xiamen University*

Corresponding Authors: chx@xmu.edu.cn, shuyu.sun@kaust.edu.sa

Simulation of flow and transport in porous media has wide applications, which include in particular the management of existing petroleum fields and the development of new oil and gas reservoirs. In this talk we will introduce a new efficient IMplicit Pressure Explicit Saturation (IMPES) scheme for the simulation of incompressible and immiscible two-phase flow in heterogeneous porous media with capillary pressure. The new algorithm is locally mass conservative for both phases and also deserves another merit that the total velocity is continuous in the normal direction. Moreover, the new scheme is unbiased with regard to the two phases and the saturations of both phases are bounds-preserving if the time step size is smaller than a certain value. We will also discuss the application of the idea of the new algorithm to develop the fully mass-conservative scheme for the multicomponent compressible flow in porous media. Some interesting examples will be shown to demonstrate the efficiency of the new algorithms.

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EG-based GMsFEM for Darcy Flow in Porous Media

Author: Huangxin Chen[1]

Co-author: Shuyu Sun [2]

[1] *Xiamen University*

[2] *King Abdullah University of Science and Technology (KAUST)*

Corresponding Authors: shuyu.sun@kaust.edu.sa, chx@xmu.edu.cn

In this talk we will introduce the generalized multiscale finite element method (GMsFEM) based on the enriched Galerkin (EG) approximation for solving Darcy flow in heterogeneous porous media. The EG method could conserve local and global fluid mass by enriching approximation space of the continuous Galerkin method with piecewise constant space. To construct the multiscale basis functions for each coarse grid element, we use the EG method to obtain the snapshot space. Only the pressure is used for approximation and the velocity can be recovered to be mass-preserving. Then the offline space is obtained by solving some local spectral problems to reduce the snapshot space. The convergence of the EG-based GMsFEM will also be shown and some numerical examples will be given to illustrate the good efficiency of the proposed method.

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Permeability prediction of fibrous porous media by the lattice Boltzmann method with a fluid-solid boundary reconstruction scheme

Author: Suguru Ando[1]

Co-authors: Masayuki Kaneda [1]; Kazuhiko Suga [1]

[1] *Department of Mechanical Engineering, Osaka Prefecture University*

Corresponding Author: ando@htlab.me.osakafu-u.ac.jp

Flows through fibrous porous media have been investigated for many decades due to significant importance in numerous industrial applications such as filtration, heat exchangers, fabric reinforcements, etc. Recently, high performance nonwoven fabrics have taken the place of traditional materials owning to the development of the production technology 1. Accordingly, a numerical tool for accurately analyzing fluid flows through nonwoven fabrics without conducting expensive or time-consuming experiments is required for designing the effective production process. Therefore, this study presents the lattice Boltzmann method (LBM) with a fluid-solid boundary reconstruction method to predict permeability of fibrous porous media.

The LBM is a computational fluid dynamics technology based on the discretized Boltzmann equation, which treats a fluid flow by the time-evolution of the distribution function for the groups of particles that move and collide on lattice nodes. Due to its discrete nature and high computational efficiency,

the LBM is efficient to investigate mesoscale flows in complex geometry such as fibrous porous media, compared to continuum-based approaches 2. In this study, the D3Q27 discrete velocity LBM model is employed. To treat fiber surfaces, the interpolated bounce-back method (IPBB) combined with an integrated fluid-solid boundary reconstruction process (fsBR) based on the CT-scanning and the boundary reconstruction method 3 is proposed. Compared to the conventional half-way bounce-back method (HWBB), the proposed method (fsBR-IPBB) employs a level-set function to represent solid surface smoothly, resulting in highly accurate calculations despite low lattice resolutions of fibers with a smooth circular cross-sectional shape. Pressure gradient and periodic boundary conditions are applied to the inlet and outlet boundaries, and remaining boundaries, respectively.

We evaluate the proposed method by comparing permeability of nonwoven fabrics obtained by numerical methods (HWBB and fsBR-IPBB) with that by experimental measurements. Nonwoven fabrics are prepared by the hydroentanglement process, which is an important industrial polymer process to produce highly entangled nonwoven fabrics. The hydroentanglement imposes high-pressure water jets to entangle and bond loose polymer fibers. Therefore, mechanical properties of fibers and water jet pressure are key factors to determine characteristics of nonwoven fabrics [4]. In this study, three types of fibers, rayon (2.2 and 3.3 dtex) and PET (2.2 dtex), are hydroentangled using two different water jet pressures (5 and 8 MPa), resulting in six types of nonwoven fabrics. The binary 3D structure data of nonwoven fabrics are acquired by the X-ray computed microtomography at a resolution of 2.16 mu;m, and then combined with HWBB-LBM and fsBR-IPBB-LBM to calculate permeability from simulated velocity fields. The results show that calculated permeability is in good agreement with measured one, and that the fsBR-IPBB is more accurate than HWBB with an error of 5.2 –8.0%. (Note that errors from measured permeability increase as the bending stiffness of fibers decreases, indicating that finer materials or highly absorbent materials such as rayon easily deform when they are exposed to water.) The relationship between permeability and porosity is found to be different from those by the Kozeny-Carman equation and its derivatives due to the highly anisotropic geometry of hydroentangled nonwoven fabrics.

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The Images Detection of Granular Fibers and Composite Materials through Multi-Windows Object Detection Method

Author: Qiaonan Li[1]

Co-author: Weifeng Liu [1]

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

Corresponding Authors: liuwf@upc.edu.cn, lqn19940321@163.com

The images detection of granular fibers and composite materials is one essential step in the production process. We can understand and calculate number of granules, diameter, fiber content and other useful information through the images detection. The accurate detection of granular fibers and composite materials will provide suggestive advice and reliable data reference for their design,

production, and subsequent utilization. Traditional images detection methods including manual measurement, binarization and connected component labeling algorithm. But these methods are complicated and tedious, it is still a great challenge to achieve high accuracy and automation level. This paper presents a multi-windows object detection method for the images of granular fibers and composite materials. In particular, it segments the image into multiple sub-regions, and each sub-region is detected by the convolutional neural network separately. The coordinate of bounding boxes in the sub-regions are converted to the original image according to its position in the original image, and then they are selected by the non-maximum suppression. We conduct experiments on collected microscopic images of granular fibers and composite materials and the results demonstrate the superiority to the traditional methods. Specifically, the proposed algorithm can obtain nearly the same performance as the manual detection, i.e. less than 5% detection error, with significant time reducing.

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Digital Core Flow Simulation and Application in Bohai Oilfield Based on Lattice Boltzmann Method

Author: Bowei Liu[None]

Co-authors: Songru Mou ; Bo Quan ; Dongdong Yang ; Wei Yang

Digital core technology has sprang up in recent years. Microscopic pore flow simulation has been widely used in Oil-Gas Field Development Engineering. Bohai Oilfield has done deep research on microscopic pore sweep degree and remaining oil state. However, data such as digital cores and thin slices of rock castings are mainly used to do static observation and qualitative analysis, lacking for rock pore flow simulation and visualization analysis. Based on data of digital cores and rock castings slices, this paper implements core skeleton extraction and pore network modeling, by using integrated image processing technologies, such as watershed algorithm and boundary tracking algorithm. It can realize rapid calculation of core porosity, and the result error is less than 4.0% compared to laboratory testing. A flow system is set up by using the lattice Boltzmann method, LBGK model / Shan-Chen model and bounce-back boundary of the non-equilibrium distribution, this system can realize the single / multi-phase flow simulation visualization of digital core in pore level. Under different displacement pressures and fluid viscosities, this can also realize 2-D and 3-D visual flow simulation, and the dynamic displacement process is more than 85% consistent with laboratory etched glass water flooding experiment . With the method in this paper, the micro-flow mechanism experiment has been started in Bohai Oilfield. Through the analysis of reservoir microscopic water flooding oil flow rule and microscopic residual oil occurrence state, it can effectively guide the microscopic residual oil to tap the potential.

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A new parallel framework for general purpose reservoir simulation with advanced discretization and linearization schemes

Authors: Longlong Li[1]; Ahmad Abushaikha[1]

[1] *Hamad Bin Khalifa University*

Corresponding Authors: aabushaikha@hbku.edu.qa, lilonglong.upc@gmail.com

As the main approach to predict flow response in the subsurface, reservoir simulation plays a vital role in risk analysis and uncertainty quantification. However, there are still many challenges since an accurate representation of strong heterogeneities requires a high-resolution grid, the representation of rock permeability may require full tensor format, the meshing of complex geological models requires unstructured grids, and the complex physical process enhances the nonlinearity of the system. All of them drastically reduce simulation efficiency and accuracy. In this work, we develop an advanced parallel framework for general purpose reservoir simulation using state of the art discretization and linearization methods. We apply the mimetic finite difference method to improve the accuracy of simulations employing full tensor permeability and unstructured grids. To represent the complex subsurface physics in a general approach, we apply mass-based formulations which can be described in an operator form employing the Operator-Based Linearization (OBL) approach. The OBL simplifies the assembly of the residual and the Jacobian significantly and reduces computational time spent on phase behavior calculations drastically. To further improve the performance of the framework, we apply massively parallel techniques via Message Passing Interface (MPI) which allocate a huge workload to the processors on a cluster. Several realistic cases implemented in this work demonstrate that the parallel framework is capable to provide accurate and efficient solutions for general purpose reservoir simulation.

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Understanding Hydraulic Fracturing Dynamic Stimulation: Dynamic Characterization and Design Considerations for Tight Porous Media

Authors: Abhijith Suboyin[None]; MD Motiur Rahman[1]

Co-author: Mohammed Haroun [1]

[1] *Associate Professor*

Corresponding Authors: abhijith.suboyin@ku.ac.ae, mohamed.haroun@ku.ac.ae, md.rahman@ku.ac.ae

Tight reservoirs in the Middle East are widely known for their extremely low porosity and permeability. Augmented by recent activities in the oil and gas industry, it can be seen that an economical and efficient hydraulic fracturing job can greatly assist in the successful development of such tight porous media.

In this study, a comprehensive investigation that deals with the quantification of changes with respect to variation in prime contributors within a traditional fracture design process is presented. This can assist to determine the distinct contributions of an element within fracture design parameters from a micro approach, as they are imperative to evaluate the fracture geometry and optimize well placement in tight porous media. After an extensive assessment, a set of natural fractures were introduced to the system and the system behavior was further investigated to identify their behavior with respect to interaction within microporous media. Based on an iterative process, the results of the constructed simulation models were analysed in depth and validated with field data.

The constructed simulation model is initially validated with conventional models along with results from field cases. With the introduction of natural fracture sets and its variation, the effect on cumulative gas production is illustrated. Overall, the results indicate the orientation and distribution of the natural fracture network are critical to achieve maximum recovery in such microporous media. The dominance of parameters such as fracture width, fracture length, proppant placement and Young's

Modulus are also illustrated in depth. To examine the associated response on long-term productivity, the results have been extended to current field practices and cases.

In addition to ultimately assisting in verification of modern best practices, this investigative approach will create a paradigm for future studies within the Middle Eastern region to assist in a simplistic prediction of fracture propagation behavior in tight porous media and its associated response to optimize treatment design. The results have also been extended along with comparisons to current field practices.

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Non-isothermal Battery Modelling

Authors: Astrid F. Gunnarshaug[1]; Lena Spitthoff[2]

Co-authors: Michael Rauter [1]; Marco Sauermoser [1]; Dick Bedeaux [1]; Preben J. S. Vie [2]; Odne S. Burheim [2]; Signe Kjelstrup [1]

[1] *PoreLab, Department of Chemistry, Norwegian University of Science and Technology, NTNU, Trondheim*

[2] *Department of Energy and Process Engineering, Norwegian University of Science and Technology, NTNU, Trondheim*

Corresponding Authors: lena.spitthoff@ntnu.no, astrid.f.gunnarshaug@ntnu.no, michael.t.rauter@ntnu.no

Temperature is known to affect ageing and performance of lithium ion batteries 1 in addition to affecting electrochemical impedance spectroscopic (EIS) measurements and modelling. Several models have been developed to describe the temperature change in batteries during operation 2. Most of these use the assumption of an isothermal cell and uniform electrolyte to describe the electric potential difference, and thus the heat production. As different parts of the battery have different resistances, heat capacities, thermal conductivities and thermal diffusivities, the assumption of an isothermal cell is unrealistic especially at high discharge as well as charge rates. In addition, the reversible heat effect will not distribute uniformly across the cell, but lead to heat absorption on one electrode and heat release on the other 3. Moreover, contributions from non-uniform electrolytes to local heat effects have been shown to be substantial [3,4].

We present a general complete battery model and show that under the assumption of uniform electrolyte distributions and isothermal conditions, we arrive at the expressions usually used in battery modelling. A simplified implementation of this model at steady state conditions in the electrolyte will be presented. The theoretical model will be elucidated with numerical examples and plots.

Acknowledgment
The authors are grateful to the Research Council of Norway through its Centres of Excellence funding scheme (project number 262644), PoreLab and the funding received for the BattMarine project (project number 281005). We also want to acknowledge ENERSENSE group at Norwegian University of Science and Technology, NTNU, for the financial support.

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Capillarity vs. Saturation in Fracture-Matrix Systems

Authors: Qi Liu[1]; Alejandro Cardona[2]; Carlos Santamarina[1]

[1] *Earth Science and Engineering, KAUST*

[2] *King Abdullah University of Science and Technology (KAUST)*

Corresponding Authors: alejandro.cardonaramirez@kaust.edu.sa, carlos.santamarina@kaust.edu.sa, qi.liu@kaust.edu.sa

Mixed fluid flow through fractured porous media has profound implications on oil recovery, CO2 geological storage, NAPLs migration and environmental remediation. The pressure difference between the non-wetting and the wetting fluids defines the capillary pressure, and depends on the degree of saturation of the wetting phase. The capillary pressure vs. saturation PS curve and the associated relative permeability trends are critical for the analysis of imbibition and drainage processes; yet, the PS function for fracture-matrix systems remains experimentally challenging.
This study advances the analysis of fracture-matrix capillary interactions. We adopt experimentally measureable capillarity-saturation data for the matrix. For the fractures, we measure the surface topography using 3D profilometry and numerically compute the evolution of the fracture pore structure under normal and shear loading; then, we model the fracture as a porous network made of interconnected pores and throats in order to estimate the evolution of capillarity-saturation with loading. Finally, the overall capillary-saturation response for the fracture-matrix system combines the measured matrix trend and the numerically computed fracture response.

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Investigation of carbonation and degradation of well cement under geologic carbon sequestration using X-ray imaging and numerical modeling

Authors: Xiuxiu Miao[1]; Liwei Zhang[2]; Yan Wang[3]; Manguang Gan[None]

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

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

[3] *State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences*

Corresponding Authors: cumtgmg@163.com, zlw_85@foxmail.com, michelle.xiuxiu.miao@gmail.com

CO2 injection well is an important structure in transferring supercritical CO2 into underground geologic formations. The matrix of the well cement contains mainly calcium silicate hydrates (C–S–H) and portlandite (CH), along with other hydrated/anhydrous phases, when in contact with CO2 saturated brine, a series of equilibrium reactions will lead to complicate structure change, including degradation and carbonation, in cement. An experiment on aqueous CO2–cement interaction in a high pressure and high temperature reactor was carried out to investigate carbonation and degradation of cement under geologic carbon sequestration conditions. X-ray imaging of pre- and post-exposure cement samples was implemented to render the 3D microstructure of the cement samples. An image processing framework was established for characterisation of the microstructure change. A finite element model based on the X-ray CT image of a cement sample was established to reveal the dissolution and precipitation equilibrium involved in the aqueous CO2–cement interaction. The resulting dissolution and precipitation map from numerical simulation was validated by the X-ray image. The carbonation and degradation behaviour related to the reactive transport of H+, HCO3-, CO32- and Ca2+ in the cement was elucidated by combined X-ray CT image and numerical simulation analysis.

Keywords: Geologic carbon sequestration; Cement carbonation and degradation; X-ray computed micro-tomography; Microstructure characterization; Reactive transport model

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An interface-tracked dynamic network simulator for two-phase flow in porous media: recent developments and results

Authors: Santanu Sinha[1]; Magnus Aa. Gjennestad[2]; Morten Vassvik[2]; Alex Hansen[3]

[1] *Beijing Computational Science Research Center, 10 East Xibeiwang Road, Haidian District, Beijing 100193, China.*

[2] *PoreLab, Department of Physics, Norwegian University of Science and Technology, NTNU, N-7491 Trondheim, Norway.*

[3] *NTNU*

Corresponding Authors: alex.hansen@ntnu.no, santanu.sinha@ntnu.no, magnus.aa.gjennestad@ntnu.no

Pore-network modeling is a computational technique to simulate multiphase flow in porous media. With this method, the porous medium is modeled by a network of pores with simplified geometries and average flow properties are used to calculate fluid transport in each pore. This technique is proved to be more computationally efficient compared to some other computational methods such as the Lattice-Boltzmann simulations when using large systems. Here, we will present the recent developments of a pore-network simulator where the displacement of fluids are carried out with a set of interface-tracking algorithms 1. It is a dynamic pore-network model which, in contrast to the quasi-static pore-network models, takes into account the effect of both capillary and viscous forces. This model was first introduced in 1998 2 to study drainage displacements in a regular porous medium and over last few decades it had been extended to incorporate irregular reconstructed pore-networks as well as to simulate the steady-state flow with different boundary conditions. We will highlight some of the recent results of two-phase flow in porous media such as the non-linearity in the steady-state rheology 3, the behavior of the effective viscosity [4] and relations between the seepage velocities 5 using this model.

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Velocity Distribution Inside the Trapping Phase at Low Capillary Number: Direct Pore-Scale Modeling

Authors: Amir Hossein Mohammadi Alamooti[1]; Qumars Azizi[1]; Hossein Davarzani[1]

[1] *BRGM*

Corresponding Authors: h.davarzani@brgm.fr, qumarsazizi@gmail.com, a.m.alamooti@gmail.com

Transport phenomena at microscale have gained great prominence in recent years since they are of significant importance in a variety of areas including enhanced oil recovery, soil remediation, and carbon storage. Understanding of multiphase flow at pore-scale, especially, the velocity distribution has been the aim of several studies (Fakhari et al. 2018; Heshmati and Piri 2018; Roman et al. 2016; Zarikos et al. 2018). However, the impacts of displacement mechanism, fluid configurations through the pore assembly as well as dynamic properties of displacement, including those incorporated in capillary number, on velocity distribution at pore-scale are less investigated.
Here, we employ filtered surface force formulation of volume of fluid method implemented in OpenFoam (Raeini, Blunt, and Bijeljic 2012) to describe and quantify the velocity distribution in the trapping phase (Shams et al. 2018). More precisely, the main aim is to understand the behavior of recirculation phenomenon (two-phase shear-induced flow) in porous media. In this regard, a simplified 2D pore-doublet-model (Heshmati and Piri 2018) is considered as the main pore assembly to simulate the pore-scale displacement at low capillary numbers. This special geometry allows examining the role of fluid configurations. The variations in direction of flow or vicinity of the solid-liquid interface to the liquid-liquid interface can modify the shear stress transmitted and distributed inside the trapping phase. This can affect the recirculation and displacement process. To do so, the optimum mesh size was selected and then the model was validated with available experimental data.
We found that regardless of the displacement mechanism, the recirculation phenomenon inside the trapping phase is created with a zero velocity zone in centroid. During the imbibition mechanism, two stagnant regions are created adjacent to the fluid/fluid interface inside the invading fluid. In the drainage mechanism, the concavity of the trapping phase at the interface results in the creation of two adjacent recirculation zones in both invading and trapping phases near the dead-end which is not along the mean direction of flow. In addition, it is found that the more the shear stress is transmitted, the more intensified recirculation is formed. Changes in interfacial tension reshape (Brackbill, Kothe, and Zemach 1992) the liquid-liquid interface resulting in the relocation of the centroid in the recirculation zone. The changes in the viscosity ratio affect not only the velocity field inside the trapping phase but also the centroid location. The injection velocity exclusively influences the values of the velocity vector (Kashid, Harshe, and Agar 2007).
We anticipate that these results can be considered as a good pioneering step for more complicated cases where the other parameters can be combined with momentum transfer such as mass and heat transfer to analyze the transport phenomena in a more specific area. Furthermore, the recirculation phenomenon can play a crucial role during the mobilization process in porous media where several forces i.e. viscose, inertia, and capillary forces are working simultaneously.

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CO2 Storage Potential in Naturally Fractured Reservoirs

Authors: Rafael March[1]; Florian Doster[1]; Sebastian Geiger[1]

[1] *Heriot-Watt University*

Corresponding Authors: s.geiger@hw.ac.uk, f.doster@hw.ac.uk, r.march@hw.ac.uk

Geological storage of CO2 is a key technology to mitigate the impact of the increasing anthropogenic CO2 emissions in the atmosphere. Naturally fractured reservoirs are ubiquitous in the subsurface, but are typically not considered for geological storage of CO2. Two major points of concern are the high conductivity of the fracture system and capillary forces that oppose the drainage of the resident brine by CO2. Fractures typically lead to fast flow of injected CO2 through the reservoir, and capillary pressure effects may prevent CO2 flow in the rock matrix, which provides larger volume and higher storage security. Thus, storage performance in naturally fractured reservoirs depends on the competition between the CO2 flow rates in the fracture system, which controls the magnitude of the forces that drive the CO2 transfer to the rock matrix, and the timescale in which this transfer occurs. In this paper, we assess CO2 storage potential in naturally fractured reservoirs by analysing the interplay between CO2 flow in fractures and CO2 transfer between fracture and matrix. Our analytical and numerical experiments are based in large saline aquifers that have been identified as potential carbon storage sites. Our results suggest that the amount of CO2 transferred to the matrix during injection in a fractured reservoir is typically of the same order of magnitude of the CO2 that is structurally stored in an unfractured reservoir; contrary to the common belief that capillary forces would prevent the transfer to the matrix. This happens because 1) fractures increases the injectivity of a formation; 2) the plume thickness in the fracture system is typically sufficient to overcome the capillary entry pressure of the matrix and 3) the timescales of matrix drainage are comparable to the timescales of CO2 flow in the fracture system. We find that naturally fractured reservoirs should not

generally be discarded as storage locations and under the right conditions they can serve as excellent storage formations.

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From open source to open workflows?

Authors: Dmitri Naumov[1]; Erik Nixdorf[1]; Haibing Shao[1]; Jörg Buchwald[1]; Karsten Rink[1]; Lars Bilke [1]; Olaf Kolditz[1]; Thomas Fischer[1]; Thomas Kalbacher[1]; Thomas Nagel[2]; Wenqing Wang[1]

[1] *Helmholtz Centre for Environmental Research –UFZ*

[2] *Technische Universität Bergakademie Freiberg*

Corresponding Authors: thomas.kalbacher@ufz.de, wenqing.wang@ufz.de, olaf.kolditz@ufz.de, dmitri.naumov@ufz.de, erik.nixdorf@ufz.de, haibing.shao@ufz.de, lars.bilke@ufz.de, joerg.buchwald@ufz.de, thomas.nagel@ifgt.tu-freiberg.de, karsten.rink@ufz.de, thomas.fischer@ufz.de

For the analysis of environmental systems more and more workflow concepts are under debate and being implemented. A key issue is seamless integration of both observation and modelling concepts - still and mostly treated in independent ways. Developing and establishing continuous workflows in environmental systems analysis integrating observation as well as modelling aspects shall help overcoming this disparity [4]. In this paper we present basic concepts of workflow development and provide examples from different applications in environmental geosciences. Technical workflows combine data integration, numerical simulation and data analysis as well as benchmarking and knowledge transfer 3. Those workflow applications easily can become very time consuming and expensive; therefore in addition to seamless information transfer between workflow modules (Figure), the efficiency of individual parts is essential. In this regard, a variety of computational methods will be developed and employed, such as complexity-reduced models, uncertainty quantification, high-performance computing, virtual reality for workflow embedding into real geographical/geological context, and data science methods such as machine learning [6]. Ideally, those workflows will be developed and deployed in a similar open-source manner as modern porous media simulators [e.g. 1,2]. This open science philosophy probably will interfere with particular interests of "workflow customers"and the advantages of open-source workflows must by advertised in a concerted way. It is also quite obvious that systems analysis works flows need to be linked to Internet-of-Things (IoT) concepts in the near future (Industry 4.0) 5 which might serve as another "pro"for clearing the way towards open source solutions.

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Impact of moisture transfer in the context of borehole thermal energy storage application

Authors: Haibing Shao[1]; Boyan Meng[2]; Bo Wang[3]; Sebastian Bauer[3]; Olaf Kolditz[4]

[1] *Helmholtz Centre for Environmental Research - UFZ*

[2] *Helmholtz Centre for Environmental Research –UFZ*

[3] *Christian Albrechts University Kiel, Competence Cente for Geoenergy*

[4] *Helmholtz Centre for Environmental Research UFZ / TU Dresden*

Corresponding Authors: haibing.shao@ufz.de, sebastian.bauer@ifg.uni-kiel.de, olaf.kolditz@ufz.de, bo.wang@ifg.uni-kiel.de, boyan.meng@ufz.de

In order to store thermal energy and use it for domestic heating, borehole arrays have been designed, with dozens, and sometime hundreds of wellbores connected with a pipe network. Heated circulating fluid will pass through each of the borehole and store thermal energy in the shallow subsurface. In this context, the boreholes are expected to exchange heat in the partially saturated vadose zone. Due to the high temperature of circulating fluid (70-90 degree Celsius), water in the vicinity of the borehole is likely to evaporate into the gas phase and migrate away. For the understanding of this coupled process, a tank experiment has been conducted in a 5x3x2 meter sand box located in the Kiel University. The thermal and moisture content sensors were embedded in the tank to record the dynamic evolution of water content and temperature. The non-isothermal two-component, two-phase process was simulated with OpenGeoSys software. Preliminary monitoring data and modelling results show that when the soil temperature is higher than a critical value, a drying-out zone will gradually develop in the vicinity of the borehole. Such critical temperature depends both on the specific soil characteristics (e.g. capillary pressure-saturation curve) and also on the initial water content. Obviously, the water vapor content in the gas phase experiences a sharp increase and leads to the expansion of the gas phase whose velocity is in the order of 10-5 m/s. Thermal conduction is still the dominating mechanism of heat transfer and accounts for more than 95% of the effective heat flux entering the storage tank. In addition, when multiple boreholes are installed with the same injection temperature, the interaction among them leads to distinct zonations of water content and consequently thermal conductivity which are different from the single borehole scenario. As a consequence, the heat storage efficiencies of individual boreholes are affected which is an important aspect for project designs in real applications.

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Structured Mini-Dunes (SMDs) as Self-Irrigation Units: A Lesson from the Sand Dunes of Arid Regions

Authors: Afrah Al-Shukaili[1]; Ali Al-Maktoumi[2]; Anvar Kacimov[1]

[1] *Department of Soils, Water and Agricultural Engineering, College of Agricultural and Marine Sciences, Sultan Qaboos University*

[2] *Department of Soils, Water and Agricultural Engineering, Sultan Qaboos University, Al-Khoud 123, Oman*

Corresponding Authors: anvar@squ.edu.om, ali4530@squ.edu.om, farah93019@gmail.com

Understanding the eco-hydrology of natural sand dunes (Maliva and Missimer, 2012) can be used in design of mini-dunes (crest ≤ 1 m) as agroengineerd "self-irrigation units". Minidunes can intercept moisture from humid air and a shallow water table (e.g. in sabkha landforms). Thus, a spot of wet low-salinity fine-textured soil can be maintained naturally in the core of the SMD's conical structure by sourrounding it with a courser layer (capillary barrier against both evaporation of the fresh water condensate in the core and ascending vertical creep of saline groundwater). In our study, we designed the SMDs trying to answer several biomimetical questions: Why and how nabkhas (minidunes reinforced by a desert shrub) act as "ecosystem engineers"i.e. maintain a mosaic of natural halophyte vegetation? Can we cultivate non-halophyte crops-ornamental plants in engineered mini-dunes over a flat sabkha land? Are pore-level models adequate in predicting unsaturated liquid and vapour fluxes in the two-component porous composite of SMD , especially in the root zone of a planted crop? We simulated by HYDRUS one-phase unsaturated flow and optimized SMD to examine the effect of the water table depth, geometry of SMD's truncated cone, its internal structure and Van Genuchten parameters of the composite on water holding efficiency. In a pilot experiment, SMD'soil was loamy shielded by 3-5 cm thick coarser sand and gravel (sizes: H= 60 cm high, W = 100 cm). Water evaporated from the water table and condensed from the wind blowing from the sea is stored and transpired by the cultivated plant. The course sand-gravel sheath (tilted and horizontal) acts as a capillary barrier similarly to ones in large dunes (Al-Shukaili et al., 2019). Understanding the water movement within the pore space of our structure will help in a smarter design of a minimum construction cost.

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3D pore scale simulation of reactive flow in catalytic filter on CT image

Authors: Oleg Iliev[None]; Torben Prill[1]; Pavel Toktaliev[1]; Robert Greiner[2]; Martin Votsmeier[3]

[1] *Fraunhofer ITWM*

[2] *Umicore AG & Co. KG*

[3] *Umicore AG & Co. KG,*

Corresponding Authors: toktaliev@itwm.fraunhofer.de, prill@itwm.fraunhofer.de, oleg.iliev@itwm.fraunhofer.de

In order to improve the performance of the exhaust after treatment system and keep reasonable complexity, the number of the used devices is reduced by enhancing wall flow particulate filters with a catalytic functionality, like selective catalytic reduction in diesel or three way catalysis in gasoline vehicles. In this case the solid matrix of the filtering media consists from inert grains and active grains. For the simulation of such devices, effective 1D models are regularly used, because they are relatively simple and fast in comparison to higher dimensional models, however the reduction of the complexity in the modeling is achieved by introducing many simplifying assumptions which in certain cases lead to reduced accuracy.

Here we present a software tool for simulation of 3D pore-scale model. The latter describes convection and diffusion in the pores and in washcoat grains, and absorption in the washcoat grains. In fact, washcoat particles are nanoporous and surface reaction (adsorption) occurs at this scale. Software tool called PoreChem 1 has been used for simulating the reactive flow at pore scale. A wall segment of a real particulate filter was used in the simulation. The three dimensional structure of the wall segment was obtained by X-ray microtomography, in which we resolved the different materials: Pores, (inert) Substrate and (active) Washcoat. The conversion (adsorbed amount) was computed for different reaction rates. The results show how the inhomogeneity of the pore size and of the washcoat distribution in the 3D system influences the adsorption processes. Effects which can not be observed in the macroscale simulations are pointed, thus confirming that the 3D pore scale models are useful in the design and optimization of catalytic particulate filters.

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Nanoporous carbon scaffolds for membrane filtration and capacitive deionization applications

Author: Arlene (Chengying) Ai[1]

Co-authors: Xiaoan Li [2]; Robert Mayall [3]; Sathish Ponnurangam [1]; Viola Birss [1]

[1] *University of Calgary*

[2] *Nanjing Momentum Materials Technologies Ltd. Co.*

[3] *FREDSense*

Corresponding Authors: robert@fredsense.com, sathish.ponnurangam@ucalgary.ca, birss@ucalgary.ca, xiaoan@momentummaterials.com, chengying.ai@ucalgary.ca

The scarcity of clean water is a major motivator of the development of more efficient water utilization and clean water production. Membrane technologies, including nanofiltration and ultrafiltration, have been widely applied in the water/wastewater treatment area. Fundamental research and commercialization efforts on new and better membranes are increasing continuously.
However, currently, nanofiltration and ultrafiltration membranes still face various problems. First, the pore sizes of most membranes are not well-controlled, which does not allow them to be used for precise particle or molecule separation. Second, most membranes experience rapid fouling issues, leading to partial or total loss of the membrane performance. Third, the majority of commercial membranes degrade rapidly at high temperatures (> 80 C), the temperature relevant to many waste water sources . Ceramic membranes can tolerate high temperatures, but they are limited by their high cost. Fourth, most polymer membranes cannot treat water that contain organic carbons or organic solvents.
A free-standing and nanoporous carbon scaffold has emerged as a powerful candidate as a next generation membrane. The nanoporous carbon scaffold, or NCS, was developed in the Birss group at the University of Calgary and is now being manufactured and commercialized by Momentum Materials Corporation, a Calgary based start-up. The NCS is a self-supported carbon material with tunable pore sizes (8 –500 nm), controllable thickness (1 –200 μm) and very good conductivity. The NCS with a pore diameter of 22 nm is able to remove solid particles as small as 10 nm. It can completely

reject E. Coli bacteria and 99.999% of viruses through a single filtration pass. Since the NCS is composed of 100% carbon, it is very stable at high temperatures (up to 600°C in air), over a very wide pH range (0-14) and in organic solvents. It has alaos been demonstrated that the NCS can fully remove solid suspensions from hexane and CCl4. In terms of membrane fouling, due to the conductive nature of the NCS, we can clean the membrane by applying periodic voltage pulses, which generate H2 bubbles from water that remove the foulants from the membrane surface. Therefore, the NCS membrane can be cleaned and recovered during water treatment at low cost.
In addition, unlike other nano/ultrafiltration membranes, the NCS can perform two functionalities at the same time. Because of its good conductivity, the NCS can act as an electrode in a capacitive deionization (CDI) cell. By using a flow-through CDI cell, the NCS electrodes can reject solid suspensions and salt ions simultaneously. The salt adsorption capacity of an NCS electrode with an 85 nm pore diameter and an 80 μm thickness is 1.4 mg/g at 2 V. Although the salt adsorption capacity is not extremely high, adsorption is extremely rapid, usually 2 to 10 seconds, as compared to 10s of minutes or a few hours for other reported carbon CDI electrodes. With these many promising properties, we anticipate that the NCS membrane will become a rising star in the water/wastewater treatment area.

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Relative magnitude of capillary over bulk viscosity resistances for NWP blobs flowing within periodic capillary tubes

Authors: Marios Valavanides[1]; Santanu Sinha[2]; Alex Hansen[3]

[1] *Unversity of West Attica*

[2] *NTNU*

[3] *NTNU, Porelab*

Corresponding Authors: alex.hansen@ntnu.no, marval@uniwa.gr, santanu.sinha@ntnu.no

We present a parametric study of the dependence of the reduced magnitude of net capillary over bulk viscosity resistances across a solitary blob driven within a periodic axisymmetric capillary tube 1 for different flow conditions. The size of the blob is arbitrary but large enough to preserve continuous contact to the tube walls. Hysteresis is considered by assuming different contact angles of the two N/W menisci (receding and advancing) [2, 3, 4]. The flow analysis implements simple Washburn type approximation for estimating Stokes resistances within the bulk flow and Young-Laplace contact line resistances across the two menisci 5. The corresponding terms are evaluated from tractable, semi-analytical expressions, for a variety of flow conditions and pairs of receding/advancing contact angles [6]. Effective hysteresis –the result of average, capillarity induced resistances- is manifested as the sum of geometric and physicochemical hysteresis terms. Geometrical hysteresis is associated to the varying pore wall conical geometry at the menisci contact lines; physicochemical hysteresis is associated to the difference between receding and advancing contact angles. The simple case of flow within straight tubes has been also examined and used as a reference.
We show that the relative magnitude of capillary over bulk viscosity resistances depends strongly on the flow rate through the capillary tube. In particular, the calculations show that, for an extended

domain of the N/W/PM system parameters and flow conditions, the net capillary pressure drop –due to contact angle hysteresis- is significantly larger that the bulk viscosity induced pressure drop.

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Core flood-on-a-chip: a study of viscoelasticity's effects on oil recovery using a foot-long micromodel

Author: Yujing Du[1]

Co-author: Matthew Balhoff [1]

[1] *University of Texas at Austin*

Corresponding Authors: balhoff@mail.utexas.edu, yujingdu@utexas.edu

Polymers such as hydroxyl polyacrylamide (HPAM) are widely used in enhanced oil recovery where they are used as an additive to water to increase the viscosity of injection fluid, therefore improving the macroscopic displacement efficiency. In addition to the capacity to increase viscosity, the viscoelasticity of HPAM polymers is also of great interest due to the non-linear flow behaviors and the complexity when coupled with a porous medium. Recent studies have shown that the contribution of viscoelasticity to the recovery enhancement is important. Macroscopic investigations (e.g., core flood) demonstrated that the residual oil after water flood can be further reduced by the injection of viscoelastic polymer solutions [Qi et al., 2016], contradicting decades of belief that polymers only improved sweep efficiency. Pore-scale studies have shown that flow instability occurs in single channel geometries and pore-networks which may relate to the macroscopic observations of improved recovery [Clarke et al., 2016; Qi 2018]. However, a definitive understanding has not been reached due to the gap between the pore-scale observations and the macroscopic outcomes.
In this work, we conduct flow experiments in a 2.5-D, foot-long heterogeneous glass micromodel core designed and fabricated in-house. The core flood-on-a-chip model has comparable length of a rock core in traditional core flood, and allows direct and in-time visualization in the pores. End effects are minimized and pore scale 3-D features are maintained. Experiments are visualized by time-lapse image capturing with a digital camera mounted above the micromodel. In each experiment, the micromodel is initially saturated with an aqueous solution (water or glycerol), then crude oil is injected until irreducible saturation is reached. The aqueous solution is injected as secondary

flood until steady state, then HPAM polymer (elastic or inelastic) is injected as a tertiary flood. After sufficient (>5 pore volumes) polymer injection, the aqueous solution used during secondary flooding is injected again until a new steady state is established in the micromodel.
We observed that, during the tertiary elastic polymer floods, the remaining oil ganglia swell and the interfaces change significantly, but no oil recovery is observed. However, during the following aqueous glycerol solution injection, 3-6% of incremental oil recovery are observed. The above phenomena are not observed when using inelastic polymer solution in tertiary flood. We hypothesize that viscoelasticity causes additional pressure at the interface between oil and polymer solutions, therefore changes the fluid distribution and the local pressure field from steady state developed from the secondary aqueous flood. When aqueous glycerol is injected again after the polymer flood, the previous immobile oil becomes mobile again. The most interesting finding is the oil recovery delay: although significant changes occur during polymer flooding, additional oil recovery is obtained only during the glycerol injection that follows the tertiary polymer flood.

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Pore-scale simulations of hydraulic properties during biomass accumulation

Author: Holger Ott[1]

Co-authors: Neda Hassannayebi [1]; Frieder Enzmann ; Johanna Schritter [2]; Martin Ferno [3]; Andreas Paul Loibner [2]

[1] *Montanuniversität Leoben*

[2] *Universität für Bodenkultur Wien*

[3] *University of Bergen*

Corresponding Authors: holger.ott@unileoben.ac.at, neda.nayebi@gmail.com, enzmann@uni-mainz.de, martin.ferno@uib.no

The accumulation of biomass in reservoirs and its impact on the hydraulic rock properties is a common issue in shallow hydrocarbon reservoirs, microbial enhanced oil recovery, subsurface hydrogen storage and conversion.
We systematically investigate accumulation and growth of microbes in the pore scale and its influence on hydraulic properties of porous media. Even though the above-mentioned issues are in principle two-phase-flow problems, the present study is limited to saturated flow conditions, which is still not sufficiently well understood.
We use microfluidics (a 2D porous media etched in a glass chip) to investigate transport and accumulation of microorganisms. The experiments were performed in two phases by using Lactobacillus Casei as model organisms. In phase 1, a bacterial suspension solution in a stationary growth phase was flooded through microfluidic chips leading to initial accumulation of microbes in the pore space. In phase 2, a nutrient (substrate) solution was injected; the supply of nutrient changes bacterial growth to an exponential mode. Biomass accumulates with a high rate in the pore space.
The presentation is focusing on numerical simulations using digital twins including the experimental information of the biomass accumulation. By solving the Stokes and the Navier-Stokes equations in the pore space, changes in flow field and the permeability with increasing biomass has been studied. Treating the biomass as solid precipitate gives a first impression on the modified permeability

and hence on the porosity-permeability relationship (K(f)), but the experimental images and flooding experiments using dyes show that accumulated biomass is (a) porous, and (b) permeable. In a sensitivity study we model the open pore space explicitly and assign a range of effective porosity and permeability to the biomass occupied pore space. In the presentation we discuss the influence of the microbial activities on the K(f) relationship and the flow field. Furthermore, we show a first attempt to correlate biomass accumulation to the initial flow field as first step towards predicting biomass accumulation.

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Effect of aging method on wettability and oil recovery from danish north sea carbonate reservoirs

Authors: Samira Mohammadkhani[1]; Jonas Folke Sundberg[2]; Ming Li[2]; Karen Louise Feilberg[2]

[1] *Danish Hydrocarbon Research and Technology Center, Technical University of Denmark*

[2] *Danish Hydrocarbon Research and Technology Center, Technical University of Denmark*

Corresponding Authors: sammoh@dtu.dk, mingl@dtu.dk, klfe@dtu.dk, jonsun@dtu.dk

In this study, the effect of different initial water saturations has been studied in core plugs from the Tor chalk formation in the Danish North Sea and the recovery response measured by core flooding experiments. Oil recovery and pressure drop curves from core flooding experiments have been compared to see the effect of initial water saturation. Salinity of injection brines at secondary and tertiary stages of flooding has been changed to investigate low salinity effect. The experiments have been conducted in small scale core flooding setup, employing shorter core plugs of 1-2 cm length. As small slices with length of less than 2 cm and standard diameter are used in these experiments, the pore volume is more than 2.5 times less than the standard core plugs. Hence the amount of materials (oil and brine) and also consumption time is lower than the long core flooding experiments. This study demonstrates that the method provides comparable results to experiments on standard cores. The core plugs were aged by a dynamic aging method, whereby the oil was continuously injected during the drainage stage until no further compositional changes in the oil was observed indicating that the core has been conditioned with surface active compounds. The oil compositional changes have been measured by infrared spectroscopy (IR) and high resolution mass spectroscopy. The effluent oil during the drainage injection was sampled in vials containing approximately every one third of a pore volume, and analyzed. The results were used to see the changes in adsorption of polar oil compounds on the rock surface.

Oil recovery and pressure drop curves from the core flooding experiments showed different trends for the same core with different initial water saturations. In the case where 21.7 % initial water saturation had been established in the core, it resulted in higher oil recovery in the secondary stage of flooding compare to the core prepared with 31.7% initial water saturation. The effect of low salinity injection was mainly observed in the earlier experiment with lower initial water saturation. The introduced aging method for the same core with different initial water saturations leads to different oil recovery possibly due to different initial wettability conditions.

The presented results investigates the importance of the interplay between wettability and initial water saturation in core flood experiments in carbonate (chalk) samples. In addition, a method to reduce the aging time is demonstrated and low salinity core flooding results are presented for both short and standard chalk core plugs.

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Impact of pair interactions on frictional fluid dynamics

Authors: Louison Thorens[1]; Knut Jorgen Maloy[2]; Mickaël Bourgoin[3]; Stéphane Santucci[3]

[1] *PoreLab - University of Oslo*

[2] *PoreLab*

[3] *ENS de Lyon*

Corresponding Authors: k.j.maloy@fys.uio.no, louison.thorens@ens-lyon.fr

Interactions between grains can take various forms and are known to have a great impact on the overall granular system. Moreover, we know from previous studies that the flow of a frictional fluid in constrained geometries evolves towards the formation of plug patterns. Which is why we propose to investigate the flow and shape of a flowing grain assembly where grains interact with each other. To do so, we used ferromagnetic beads, for which pair interactions can be tuned, placed in a narrow tube where the liquid was slowly drained out. Firstly, we addressed the role of the interactions on the triggering of an accumulation ("bulldozing") instability. Secondly, we studied the impact of these interactions on the final pattern of plugs along the tube. Our model expanded the previous cases by considering the tuning of the Janssen effect by the introduction of the grain-level interactions

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Expanding the role of pore-scale models to capture the multi-scale evolution of porous media

Authors: Sergi Molins[1]; Hang Deng[1]; David Trebotich[1]; Carl Steefel[1]

[1] *Lawrence Berkeley National Laboratory*

Corresponding Authors: hangdeng@lbl.gov, smolins@lbl.gov

Understanding the geochemical evolution of porous media is essential for many subsurface energy applications, including subsurface storage, shale gas production, fracking, CO2 sequestration, nuclear waste storage, and geothermal energy extraction. Both mineral composition and the pore-scale geometry play a significant role in this evolution.

Pore-scale models make it possible to resolve the porous media geometry explicitly in three dimensions and solve for flow and reactive transport within the pore space. Among other processes, these models can capture the channelization of the flow path due to dissolution in transport limited conditions. However, even with high performance computing, pore-scale models are still limited in their ability to treat fine-scale heterogeneity that falls below the resolution of the discretization.

We have extended a pore-scale model (Molins et al., 2012, 2014, 2017; Trebotich et al., 2014) by combining it with a porous continuum model (Molins et al., 2019). In this approach, the porous continuum model is used to capture the relevant processes in areas of the domain where resolution requirements would make the use of a pore-scale model unfeasible, while maintaining a pore-scale characterization elsewhere

In this contribution, we focus on the ability of this novel approach to capture the evolution of the media as a result of geochemical reactions. That is, two types of evolution are considered. One that applies to the continuum model component where dissolution/precipitation reactions result in the evolution of porosity. Another one that applies to the pore-scale model component where the geometry of the domain is changing with dissolution/precipitation. The resulting model is applied to the simulation of CO2 attack in fractured cementitious media.

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Failure mechanism of kerogen by molecular dynamics simulations in relation to hydraulic fracturing in organic-rich shale

Author: Tianhao Wu[1]

Co-author: Abbas Firoozabadi [2]

[1] *Reservoir Engineering Research Institute (RERI)*

[2] *Reservoir Engineering Research Institute; Rice University*

Corresponding Authors: tianhaowu.pku@gmail.com, af@rerinst.org

Hydrocarbons in organic-rich shale formations are one of the most important unconventional resources. Hydraulic fracturing is the common stimulation method to create fractures in shale formations for oil and gas production. The failure mechanism of fracturing and mechanical properties of shale media are often investigated by the uniaxial/triaxial compression tests and Brazilian tensile tests with shale core samples. In consideration of the difficulties in the experiments, microscopic simulations have been given much attention to gain insights into the mechanisms.
In this study, we provide a systematic study on the failure mechanisms of kerogen from organic-rich shale by molecular dynamics simulations. We construct three types of kerogen matrix, including type I, type II, and type III. The process of compression and extension at various stress conditions are simulated. The results indicate that the kerogen matrices show ductile behavior, but the three types have significantly different tensile failure modes. The Mohr–Coulomb failure criterion and tensile strength criterion can describe the failure envelop of the kerogen matrix very well. The kerogen matrices have smaller Young's modulus, compressive strength, and tensile strength than typical minerals. Our work reveals that kerogen is a potential weak component in shale, and the fractures

may initiate and propagate around kerogen aggregates. The effects of different fracturing fluids, including H2O and CO2, are also examined. This work sets the stage for investigating the complex mechanisms of hydraulic fracturing in shale at pore-scale.

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Low Salinity Water-flooding in Chalk Core Samples from a Danish North Sea Reservoir

Authors: Rasoul Mokhtari[1]; Benaiah Anabaraonye [2]; Karen Louise Feilberg[2]

[1] *The Danish Hydrocarbon Research and Technology Centre*

[2] *The Danish Hydrocarbon Research and Technology Centre (DHRTC)*

Corresponding Authors: klfe@dtu.dk, bana@dtu.dk, rasoulm@dtu.dk

Chalk reservoirs, due to their high storage capacity and very low permeability, is one of the most interesting cases for reservoir engineering research on carbonates. They show various fluid-rock interactions because of their active porous media as well as fluid-fluid interactions especially when they become exposed to low salinity water and a reactive crude oil. This research aims to investigate the effect of brine composition, injection scenario and temperature on oil recovery during low salinity water flooding in chalk core samples from a Danish North Sea reservoir. In addition, the mechanisms governing oil-brine-rock interactions are investigated by analyzing effluent samples and interfacial tension (IFT) measurements. For this purpose, by means of computed tomography (CT) results, homogenous chalk core samples (without any open fractures) were selected. These cores were saturated with reservoir fluids and aged at reservoir conditions for approximately three weeks. Several synthetic brines (including formation water, seawater and diluted seawater) were introduced through different injection scenarios into the aged cores at reservoir conditions. Brines used in this study were equilibrated with calcite at room temperature to minimize the effect of rock dissolution on oil recovery. Insights into the role of brine chemistry was obtained through effluent analysis performed using ion chromatography and ICP-OES. IFT measurements were conducted using a pendant drop method to quantify the extent of brine-oil interactions at reservoir conditions.
Results showed that diluted seawater (DSW) has the most significant effect on oil recovery when injected at secondary stage. Beyond the tertiary stage, no further oil production is observed, neither with changing the brine nor with increasing the temperature and flow rate. It is worth mentioning that it takes time for DSW to show its effects on production when it is injected at tertiary stage. Rock dissolution was observed at these experimental conditions, even though brines were equilibrated with calcite at room temperature. The extent of rock dissolution increased both with temperature and decreasing brine salinity. Ion chromatography results suggest that incubating the core with DSW for a period of 48 hours could promote a multi ion exchange (MIE) mechanism which leads to additional oil production. Further, chemical analysis of the composition of produced oil has been performed to identify changes in surface-active polar components. Since this study is conducted on reservoir materials from a Danish chalk reservoir, for which there is a lack of data in the literature, it supplies a significant body of data for low salinity recovery in chalk as well as investigation of the recovery mechanism. In addition, complete analysis of core effluents –brine and oil –elucidates rock-brine-oil interactions during coreflooding.

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Minkowski measure fields as basis for rock-typing and upscaling

Authors: Han Jiang[None]; Christoph Arns[1]

[1] *Prof*

Corresponding Authors: c.arns@unsw.edu.au, hanjiang_ss@163.com

The characterization of reservoir rock is crucial for the appraisal of oil and gas reservoirs. Heterogeneity of reservoir rocks exists even down to the millimeter scale, posing significant difficulties for the derivation of petrophysical properties and cross-correlations. The advancement of X-ray CT technology offers both a view of the heterogeneous internal structure of rock samples and a platform for pore scale characterization of porous media. Intrinsic to the characterization of heterogeneous samples is the competing objectives of covering a large field of view and maximizing resolution to resolve important pore-scale details controlling transport properties. This leads to the need of upscaling methods targeting the pore scale; introducing pore-scale rock-typing methods promises to lead to an efficient workflow under such circumstance.

We introduce in this work a robust method to classify heterogeneous porous structures in 3D utilizing fields of morphological properties combined with a Gaussian mixture model for data clustering. Furthermore, we introduce a 3D rock-type sampling scheme to efficiently characterize the rock-types and demonstrate the homogeneity within rock-types, leading to representative characteristic values and trends for each rock-types and physical property. We compare petrophysical properties based on 1D rock-type classifications to the introduced 3D scheme for laminated sandstones and demonstrate the superior partitioning of petrophysical properties (permeability, electrical conductivity, critical diameter of percolation) by the 3D scheme. Utilizing this rock-typing approach leads to significant reductions in computing petrophysical properties. Furthermore, spatial characteristics of the rock-type distributions are immediately accessible. Finally, we test the classification scheme by comparing upscaled effective properties against whole-sample direct calculation of effective properties.

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Evolution of reaction rates in natural porous media stemming from coupling of pore-space heterogeneity, multi-species transport and reaction reversibility

Authors: Thomas D.S. Oliveira[1]; Martin Blunt[1]; Branko Bijeljic[1]

[1] *Imperial College London*

Corresponding Authors: m.blunt@imperial.ac.uk, thomas.oliveira14@imperial.ac.uk, b.bijeljic@imperial.ac.uk

Reactive transport of solutes in porous media is encountered in many applications, such as contaminant transport and remediation in subsurface, acidization to enhance permeability in oil recovery, and packed bed reactors in chemical engineering. A principal outstanding problem in subsurface reactive transport is to determine the effective reaction rates from the pore-scale upwards. This is of key importance in highly heterogeneous natural porous media such as carbonate rock. Carbonates are known to have a significant portion of their pore space as micro-porosity, which may lead to a very wide distribution of local velocities, increasing transport heterogeneity that affects mixing and ultimately reaction. Hence, there is a need for a systematic methodology that can identify and quantify the impact of physical and chemical heterogeneity on the reaction rates. Moreover, in many problems additional complexities arising from coupling of multispecies transport and reaction reversibility need to be accurately addressed.
We develop a new methodology termed Screening Pore-Scale Imaging and Modelling (SPIM) that can be used to predict the fluid/solid reaction rates based on the systematic characterization of both physical and chemical heterogeneity in multi-mineral systems [1-3]. Physical heterogeneity of the rocks is classified in accordance with the velocity distributions obtained by numerical flow simulation on dry micro-CT images. Spatial distribution of chemical heterogeneity is also provided from the images. Performing and analyzing coreflooding CO2/brine/carbonate experiments, we show that mineral reaction rates are an order of magnitude lower than the corresponding batch rates due to mass transfer limitations. We introduce a new metrics quantifying coupled reactive transport behaviour, which describes proximity of reacted minerals to the fast channels and slow regions. Overall, a higher degree of physical (initial pore structure and associated velocity field) and/or chemical (intrinsic reaction rates and mineral distribution) heterogeneity promotes the preferential channelling effect, as opposed to uniform dissolution.
Furthermore, we simulate 3D multispecies fluid/fluid reversible reactive transport [4] in a micro-CT image of carbonate rock that entails spatially resolved information on connected micro-porosity. Direct numerical simulation of Darcy-Brinkman 5 and advection-diffusion transport equations are coupled to a general geochemical model [6]. We demonstrate salient features of mixing and reaction arising as a result of intricate pore space heterogeneity. We show that evolution of rates of formation and consumption is species-dependent, and highly distinct in macro- and micro-porosity. Well-mixed regions result in asymptotic reaction rates. In contrast, incomplete mixing leads to transient and, for some species, even non-monotonic reaction rate behaviour.
Overall, we conclude that reactive behaviour is simultaneously influenced by pore space heterogeneity, multispecies reactive transport, and reaction reversibility. This means that for complex reversible reactions in heterogeneous porous media, species-specific behaviour needs to be examined for an accurate determination of reaction rates.

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Field trials on Microbially Induced Desaturation and Precipitation for liquefaction mitigation

Author: Leon van Paassen[1]

Co-authors: Chen Zeng [2]; Caitlyn Hall ; Elizabeth Stallings Young [1]; Diane Moug [3]; Arash Khosravifar [3]

[1] *Arizona State University*

[2] *Huazhong University of Science and Technology*

[3] *Portland State University*

Corresponding Authors: egstalli@asu.edu, karash@pdx.edu, caitlyn.hall@asu.edu, dmoug@pdx.edu, leon.vanpaassen@asu.edu, zengchen@hust.edu.cn

Microbially Induced Desaturation and Precipitation (MIDP) can be used as ground improvement method. MIDP involves bio-stimulation of indigenous nitrate reducing bacteria to generate nitrogen gas by reducing nitrate. Biogenic gas production desaturates the soil, which dampens pore pressure build up during earthquake loading. At the same time these organisms oxidize organic matter producing inorganic carbon, which precipitates in presence of dissolved calcium as calcium carbonate minerals. Formation of calcium carbonate minerals cements the soil and increase strength, stiffness and dilatancy. One of the advantages of MIDP is that all substrates are soluble and can be injected at low pressure over large distances in relatively fine-grained granular materials. Hence MIDP can be used to stabilize soils with minimum disturbance underneath existing structures. If the substrates are adequately balanced there are no adverse side-products of the biochemical conversion. Where desaturation through biogenic gas production requires only a single treatment and occurs after several days, the trapped gas may not be permanent. Sufficient cementation with CaCO3 requires several treatment cycles, but results in a more durable stabilization.
Here we present the results and lessons learned from the field trials on MIDP that were performed in Toronto (ON) in Canada to improve slope stability and enable construction of bio-engineered embankments for the rivitalization of the Don River Delta into lake Ontario and submerged slopes and in Portland (OR) in the United States to reduce susceptibility of earthquake induced liquefaction. AT both sites soils predominantly consisted of sandy silts with some silty sand lenses. Monitoring included seismic cone penetration and pore pressure dissipation tests before and after treatment. Cross-hole seismic pressure and shear wave velocity measurement, flow rates, and groundwater sampling and analysis to determine substrate and product concentrations and electrical conductivity and electrical conductivity and volumetric water content using downhole sensors during and after treatment, and a 2D numerical model was developed to design treatment protocol and allow for improved interpretation of the monitoring results. Results indicate that MIDP can be stimulated and monitored in situ, but the heterogeneous soil profile, and large amount of fine-grained soils caused preferential flow through thin sand layers and possibly hydraulically induced fractures, which limited treatment efficiency. The numerical model proved sufficiently capable to interpret the monitoring results and provide predictive simulations to design and optimize treatment procedures for future applications.

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Ripening of Residual Bubbles in Porous Media: Thermodynamic Stability and Implications in CO2 Sequestration

Authors: Ke Xu[1]; Yashar Mehmani[2]

[1] *Massachusetts Institute of Technology; Peking University*

[2] *Stanford University*

Corresponding Authors: yashar.mehmani@gmail.com, xukethu@mit.edu

Capillary trapping has long been regarded as hydrodynamically stable, as capillary forces tend to dominant over viscous and buoyancy forces at the pore scale. As a result, researchers have been trying to maximize capillary trapping for CO2 sequestration to avoid formation of unfavorable gas cap. By contrast, the thermodynamic stability of trapped bubbles has been ignored until recently. Henry's law tells us that partially miscible bubbles dissolve into the surrounding liquid and diffuse down chemical potential gradients. The processe leads to a re-distribution of trapped bubbles, even in the absence of hydrodynamics, until the global free energy of the system is minimized.

We first study bubble ripening experimentally within homogenous porous media and in the absence of external fields. We show that while classical Ostwald Ripening is unstable within bulk fluids, resulting in collection of all gas a single large bubble, it does lead to stable configurations when confined within a porous medium. The stabilization is due to the non-monotonic relationship between the capillary pressure and volume of a confined bubble.

We then focus on ripening in the presence of an external field, such as gravity, which is relevant in the context of geologic CO2 storage. We show that gravity contributes an additional term to the chemical potential gradient and can, over long times (several thousand years), lead to the coarsening of bubbles at the top of a geologic formation. The implication is that, under a worst-case scenario, an overlaying gas cap can form underneath the cap rock which increases leakage risks. We identify the controlling factors of this process by first developing a simplified pore-scale model correspond to a pore doublet followed by upscaling it into a continuum equation. Macroscopic simulations over the full thickness of typical candidate formations for CO2 storage reveal that the time-scale of ripening is on the order of that for mineral trapping.

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Experimental Investigation on the Effects of Ion Type/Valency and Ionic Strength of Formation Water on Rock-Fluid Interactions during CO2 Geological Storage

Authors: Shima Ghanaatian[1]; Omid Shahrokhi[2]; Susana Garcia[1]; M. Mercedes Maroto-Valer[1]

[1] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, UK*

[2] *Heriot-Watt University*

Corresponding Authors: o.shahrokhi@hw.ac.uk, m.maroto-valer@hw.ac.uk, sg116@hw.ac.uk, s.garcia@hw.ac.uk

Abstract

Carbon dioxide (CO2) geological storage is a promising strategy to reduce CO2 anthropogenic emissions and global warming 1. It is critical, therefore, to ensure the security of long-term CO2 storage and understanding the intricate rock-fluid interactions happening at micro/pore-scale following CO2 injection. Since sandstones are usually selected for the CO2 sequestration process 2, a comprehensive understanding of the reactivity of sandstones is crucial. Both the ionic strength and ion type/valency of the formation water have been reported as key parameters in ascertaining different geochemistry aspects of rock-fluid interactions 2. However, to the best of the authors'knowledge, the effects of these parameters on reservoir rock dissolution phenomena are not well understood. This is because most studies use solely NaCl for the preparation of synthetic brines and compare NaCl brines with deionised water for illustrating the effect of different salinities [3, 4].
Therefore, the aim of this study is to improve our understanding on the effects of ionic strength/ion valency and the mechanisms of rock dissolution at aquifer conditions relevant for CO2 storage. This research work focuses on the four most frequent alkali and alkaline earth cations present in formation water, namely Na+, K+, Mg2+, and Ca2+, at various ionic strengths. Hydrothermal batch experiments were conducted at 130 bar and 60℃ using Berea sandstone for the duration of 840

hours to simulate the conditions of CO2 storage in deep saline aquifers. Various micro-scale imaging techniques, including micro-computed tomography (μ-CT), Environmental Scanning Electron Microscopy-Energy Dispersive X-ray Spectroscopy (ESEM-EDS) were employed to understand how different chemistries of formation water can affect the mineralisation of injected CO2. μ-CT facility scanned 10×5×5 mm core plugs to retrieve pore structure and the spatial distribution of minerals at pre/post-experiment conditions. The μ-CT images were acquired at 82 kV and 72 μA and the voxel size of the 3D reconstructed geometry is 4μm×4μm×4μm, while the initial porosity is 0.18.
In addition to the displacement of clay particles, the results from pore-scale imaging using μ-CT and ESEM-EDS indicated both dissolution of primary minerals (e.g. calcite and feldspars) and precipitation of secondary minerals (mainly iron(III) oxide), while smaller pore throats are more vulnerable for mineral precipitation. Furthermore, through a comparison of the post-experiment images, it could be inferred that a stronger ionic solution leads to a higher degree of reactivity.
In conclusion, this study provides new insights into the roles of ions/ionic strength of aqueous phase and mechanisms of water-rock interactions during CO2 geological storage. The results demonstrate that rock-fluid reactivities increased with ionic strength and every single cation is effective in determining the rock-fluid interactions.
Figure 1 depicts the micro-CT and ESEM-EDS results of the reservoir rock dissolution at pore-scale.

Acknowledgments
This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (MILEPOST, Grant agreement no.: 695070). This paper reflects only the authors'view and ERC is not responsible for any use that may be made of the information it contains.

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Bubble Deformation by Pore-Throats Modifies Dissolution in Porous Media

Authors: Yu Qiu[1]; Ke Xu[2]

[1] *Massachusetts Institute of Technology*

[2] *Peking University; Massachusetts Institute of Technology*

Corresponding Authors: xukethu@mit.edu, yuqiu@mit.edu

Capillary pressure (P_c) posed on a bubble renders additional gas solubility in surrounding liquid as shown by Henry's law. This additional solubility increases the total concentration gradient which drives gas dissolution, therefore modifies the dissolution kinetics. Specifically, when a bubble volume (V_{bub}) is in very small that P_c dominates over liquid pressure (P_o), or when the liquid is very closed

to saturated gas concentration, P_c can be determinative. These conditions are common in oxygen supply in near-surface ecosystem and CO2 dissolution trapping sequestration.

P_c - V_{bub} correlation for a bubble trapped in porous media can be very different from that for a bubble in open space, as shown in [Xu et al., PRL, 2017; Xu et al., GRL, 2019]. Pore-throat geometry regulates the bubble into a non-spherical shape, that P_c is no longer a monotonically decreasing function of V_{bub} as that of a spherical bubble in open space. The pore-throat confinement forces the bubble to have much larger capillary pressure than a spherical bubble of the same volume. As a consequence, classic models applying the assumption of spherical bubble and corresponding capillary pressure during dissolution may be invalid

We verify by numerical modelling that this modified P_c - V_{bub} correlation due to pore geometry confinement does have non-trivial effects on the bubble dissolution rate. Dissolution process is significantly accelerated leading to much shorter bubble lifetime. The scaling between bubble life time and bubble volume is also modified. Specifically, for a ganglion trapped in microfractures with large aspect ratio or in multiple pores, the dissolution rate of this ganglia can be orders of magnitude accelerated than spherical bubble in same condition and same initial size.

As a conclusion, it is necessary to include modified P_c - V_{bub} correlation due to pore geometry confinement in to modeling of bubble dissolution. Furthermore, this study implies the necessity to take bubble deformation into consideration also for other physical process where capillary effects are significant.

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Wetting dynamics of nanoliter water droplets in nanoporous media

Authors: Bin Pan[1]; Christopher Clarkson[2]; Marwa Atwa[3]; Chris DeBuhr[2]; Amin Ghanizadeh[2]; Viola Birss[3]

[1] *Department of Chemical and Petroleum Engineering, Department of Geoscience, Department of Chemistry, University of Calgary*

[2] *Department of Geoscience, University of Calgary*

[3] *Department of Chemistry, University of Calgary*

Corresponding Authors: aghaniza@ucalgary.ca, birss@ucalgary.ca, marwa.atwa@ucalgary.ca, cdebuhr@ucalgary.ca, clarksoc@ucalgary.ca, bin.pan1@ucalgary.ca

The study of wetting phenomena in nanoporous media is important for understanding various natural processes and for various other technological advancement, e.g., in water infiltration, unconventional hydrocarbon recovery, and ink printing. However, access to relevant experimental data is quite scarce in the literature and the underlying imbibition dynamics are still uncertain. The primary objective of this work is to investigate spontaneous imbibition of nanoliter-sized droplets into a well-defined nanoporous carbon scaffold (NCS), which has highly controllable wettability and pore geometry properties. In this work, a series of sessile nanoliter water droplets (2.8 to 33.6 nL) were generated using a recently-developed micro-injection technique and placed onto an NCS surface. The wetting dynamics of these droplets were then monitored using an environmental scanning electron microscopy (ESEM).

The measured apparent contact angle (i.e., θ_apparent) decreased continuously from >90° initially to 0°, which demonstrates a shift in surface wettability due to imbibition into nanopores. For the duration of the contact angle measurements, the droplet volume decreased almost linearly with time and the contact line remained pinned. A theoretical model was developed to characterize these imbibition dynamics. The predicted advancing contact angle inside the NCS pores (θ_advancing) using this model is around 89°, a significant difference from θ_apparent on the NCS surface. These results are the first to demonstrate that spontaneous imbibition occurs on a hydrophobic surface, which is attributed to capillary condensation. In addition, it was observed that a larger pore size leads to a larger initial θ_apparent but a smaller imbibition rate, while a larger droplet size gives a larger initial θ_apparent. The cosine of the initial θ_apparent scales linearly with the reciprocal of the equivalent spherical radius (1/R_sphere), where R_sphere ranges from 20 μm to 200 μm. The results of the systematic experiments conducted in this work are important for understanding the nature of nanoliter droplet wetting dynamics at the nanoscale, and they could also have significant implications for understanding wettability in other natural/synthetic nanoporous media.

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Automation of flow simulation in porous media

Authors: Masa Prodanovic[1]; Honggeun Jo[1]; Michael Pyrcz[1]

[1] *The University of Texas at Austin*

Corresponding Authors: mpyrcz@austin.utexas.edu, honggeun.jo@utexas.edu, masha@utexas.edu

3D spatial geometry details in combination with simulations allow investigating non-linear flow and mechanical phenomena for both understanding and decision-making purposes and from pore/grain length scale which is imaged with constantly increasing level of detail to the reservoir-scale description of subsurface formations. The barrier to scientific progress is not acquiring data, however, but automation: enabling and maintaining a data sharing and computational environment that links curated data across spatial and temporal scales and simulations in an efficient way.

In this presentation, we touch upon the nexus of data and efficient simulation, having deep learning approaches in mind that require large amount of data to train. We review Digital Rocks Portal (https://www.digitalrocksportal.org) platform for curation and basic analysis of microstructure images, and introduce workflows that reuse its data for simulation of flow properties in an automated fashion. We then present application of convolutional neural network (CNN) algorithms to predicting permeability and contrast input and training required for simulation on both pore scale (where digitized image is required) and larger scale (where permeability map is required). Once CNN is trained, it cuts down 8+ hours simulation time down to seconds. We finally comment on the reliability of results when used in new subsurface context as well as ability to explain erroneous outputs.

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Validating machine learning permeability prediction

Author: Matthew Andrew[1]

[1] *Carl Zeiss X-ray Microscopy*

Corresponding Author: matthew.andrew@zeiss.com

One of the biggest challenges in flow and transport in geological porous media is that of scale. Frequently the resolution required to describe a pore structure comes at the expense of a field-of-view representative of rock heterogeneity. This challenge is particularly pronounced as the computational determination of effective flow and transport properties (e.g. permeability, diffusivity or effective conductivity) has required 3D imaging, imposing both technological and practical limitations on the scale of examination. 2D techniques allow for the examination of much larger length scales, but such data cannot easily be translated into effective properties. The past 10 years have seen an explosion in the availability of open source machine learning tools, allowing for an in-depth multivariant analysis of porous media structure and new approaches for the prediction of flow and transport properties.
Recent work1 has shown that machine learning based techniques can be used to predict permeability using only 2D data with a mean-square-fractional-error (MSFE) of <25%. We use this technique to analyze permeability predictions on 4 samples, two from micritic carbonate microporosity, and two from granular sandstones, imaged using a range of 2D and 3D imaging techniques, including micro-CT, nano-CT, Scanning Electron Microscopy (SEM) and automated optical petrography.
Micritic carbonate microporosity samples were extracted from a sample of Estaillades Limestone. A polished optical thin-section of the sample was scanned at 20X magnification using an automated petrographic microscope. The microporous grains were targeted for high (20nm) resolution scanning using an SEM. Two regions from microporous grains extracted using a femto-second laser, then scanned at high (65nm) resolution using a nano-CT. The top slice of the 3D CT data spatially correlated with the light and electron microscopy data from the same region. Granular sandstone samples were extracted from two samples of Berea Sandstone. Two 1"diameter cores were imaged at high (1.6μm) resolution using a X-ray microscope. Polished thin-sections were prepared for each sample and scanned using automated petrography.
Each sample therefore had a high-resolution 3D volume, spatially correlated with a scalable high resolution 2D image of the same region. For each sample permeability predictions were made from the 3D CT data using both multivariant prediction1 and Geodict software (Math2Market Gmbh.). Multivariant predictions were also made from the (2D) overlap region between the CT data and the SEM / optical petrography data. The multivariant predictions and the full-physics simulation predictions agreed to within the 25% MSFE shown by 1. The overlapping single-slice predictions from both CT data and SEM/optical petrography data agree extremely well (around 5% difference) for all samples. The single slice predictions agreed reasonably well with the full volume predictions, with better predictions made for sandstones (<25% error) than carbonates (around 50% error). This discrepancy is likely due to the greater level of heterogeneity within the carbonate microporosity.
The validation of the use of 2D imaging techniques to predict flow properties allow for much larger spatial length-scales to be analyzed at the pore-scale, and potentially enabling direct upscaling from the pore to core scales.

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Pore system evaluation of a bi-modal carbonate rock using a suite of low field NMR and microCT techniques

Authors: Jun Gao[1]; Ahmad AlHarbi[1]; Hyung Kwak[1]

[1] *Saudi Aramco*

Corresponding Author: jun.gao@aramco.com

The characterization of the complex carbonate pore systems and their effects on the oil/water flow remain as challenges of the study on flow through porous media. The pore size distributions may cover the range of several orders of magnitude. The sub-pore systems and their connectivity are essential to the microscopic sweeping efficiency during water and EOR floods. Conventional techniques such as MICP and thin section can only give some static quantities without their implication to the oil/water flow therewithin. Various NMR techniques are employed over the years to reveal both the static and dynamic properties of a bimodal carbonate. The current study utilizes more NMR and microCT techniques in addition to the previous T2 measurements during miscible D2O/H2O displacement to further differentiate the dead-end and inaccessible pore fractions.

The previous studies in this typical bi-modal carbonate focused on the analysis of D2O/H2O displacement using the capacitance model for convective-dispersive parameters and the displacement efficiency in both mico and macro pores to infer the possible parallel and series configurations. The current study continues by introduction of new 2D T2-store-T2 and displacement propagator (displacement probability distributions through APGSTE PFG NMR) measurements. 3D images of different voxel resolutions (multi-scale) from microCT are employed to differentiate the micro pore types and their spatial connection to the macro pores. All measurements are performed in the same rock, and their results compared.

Two types of micro pores are identified for this bi-modal carbonate: dead-end and inaccessible. For rocks with mainly dead-end micro pores, the flow fraction is close to 1 from capacitance model and displacement efficiency, there are off-diagonal peaks in T2-store-T2 map, and the flow peak of propagator can be fitted by a Gaussian. On the contrary, for rocks with mainly inaccessible micro pores, flow fraction is less than 1, off-diagonal peaks are not apparent, and flow peak cannot be fitted by a Gaussian. This distinction from all techniques indicates the different micro pore connectivity to the main flow channel (macro pores). Water flooding performance is expected to be related to the connectivity and EOR agents can be better designed to mobilize the oil with known connectivity. More petrophysical properties can be better correlated for this complex carbonate based on the new characterization.

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Numerical simulation of convective mixing in geologic carbon sequestration applications

Author: Anna-Maria Eckel[1]

Co-author: Ronny Pini [1]

[1] *Imperial College London*

Corresponding Author: a.eckel18@imperial.ac.uk

In the context of carbon sequestration, solubility trapping of carbon dioxide (CO_2) into reservoir brine is seen as one of the key mechanisms for securely storing significant quantities of CO_2 in deep saline aquifers on a long term. The molecular dissolution of CO_2 into the brine causes a slight increase in the solution density, creating a gravitational instability. As a result, density-driven convection is established in the form of a characteristic finger-like pattern, which accelerates the mixing process and the dispersal of the CO_2 rich brine. This causes much higher dissolution rates for CO_2 in comparison to rates from diffusion alone. However, making reliable estimates of the rates of CO_2 dissolution in geological CO_2 storage sites is challenging because the time- and length-scale of this mixing process are largely uncertain.
A CFD-FEM model that simulates the convective mixing in a two-dimensional porous media over a

range of Rayleigh numbers was developed using COMSOL Multiphysics®. While previous studies have focused almost exclusively on evaluating the dissolution flux, in this work we have extended the analysis to include various statistical measures of mixing that make use of the local spatial structure of the concentration field in the medium. In particular, both the dilution index and the spreading length confirm a significantly accelerated mixing process, with a power-law scaling that transitions from diffusive mixing (power-law exponent of 0.5) to convective mixing (exponent of 1). This transition is also confirmed by a rapid decrease in the so-called intensity of segregation, which quantifies the decay of concentration variance in the medium. The non-dimensional mass flux in terms of the Sherwood number reveals a linear scaling with high Rayleigh numbers, which agrees with experimental and numerical studies from the literature for convective mixing driven by heat rather than dissolution.
This numerical framework provides a solid starting point for the systematic evaluation of the mixing process in more complex (and realistic) situations, including those characterised by structural heterogeneity.

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Redistribution of residually trapped CO2 by Ostwald ripening due to capillary heterogeneity

Authors: Yaxin Li[1]; Charlotte Garing[2]; Sally M Benson[1]

[1] *Stanford University*

[2] *University of Georgia*

Corresponding Authors: smbenson@stanford.edu, charlotte.garing@uga.edu, yaxinl@stanford.edu

Geological CO2 sequestration in deep saline aquifers is proposed to be an important tool for reduction of industrial CO2 emissions. Aiming at isolating CO2 from the atmosphere over thousands of years, long-term security of injected CO2 in the subsurface is of great significance. One of the trapping mechanisms that reduce CO2 mobility is referred to as residual trapping. Carbon dioxide injected into a saline aquifer forms a large plume and migrates both upward and laterally. At the trailing edge of the plume, CO2 is disconnected into ganglia by imbibition of formation brine and trapped in pore spaces by capillary forces. Typically, residually trapped CO2 is assumed to be permanent in numerical simulation, and yet little evidence supports this assumption. We have found that Ostwald ripening may serve as a mechanism that could redistribute and potentially remobilize residually trapped CO2.

Previous research has found that trapped ganglia may be present at different capillary pressures and out of equilibrium. This capillary pressure gradient may result in a CO2 concentration gradient in the aqueous phase that initiates CO2 diffusion among ganglia. At equilibrium, the ganglia approach an equilibrium capillary pressure, and their volumes are changed even if the ganglia are completely trapped. More interestingly, the equilibrium capillary pressure varies in different porous media and is roughly at the same order of the entry pressure. Therefore, we propose a new scenario of Ostwald ripening at the continuum scale that potentially redistribute residual CO2. Two homogeneous porous media with different capillary pressure curves are put into contact at their residual CO2 saturation. The capillary pressure will be different between the two media, which initiates a diffusive flux of CO2 in the aqueous phase from the high capillary pressure medium to the low capillary pressure medium. At equilibrium, the residual CO2 will redistribute, resulting in a CO2 saturation increase in the low capillary pressure medium, which may increase the potential risk of remobilization of residually trapped CO2.

Therefore, evaluating the time scale of residual CO2 redistribution due to Ostwald ripening is crucial to determine its significance. We develop an approximate solution for predicting the time scale

of Ostwald ripening at any stage during equilibration. The solution has been validated to be highly accurate by detailed numerical simulation over a wide range of parameters that are relevant to conditions of geological CO2 sequestration. It is shown that for millimeter-scale models, the equilibration can take months to years, while it may take thousands of years or longer in meter-scale models. In general, Ostwald ripening is a very slow process at the reservoir scale. Furthermore, we develop an "analogous retardation factor"to give a rigorous mathematical explanation of the significantly longer time scale compared to a single-phase diffusion problem (no separate-phase CO2). The existence of separate-phase CO2 retards the equilibration roughly by five orders of magnitude.

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DoE*-based history matching as a method for uncertainty quantification in THM(C) models of clay

Authors: Jörg Buchwald[1]; Olaf Kolditz[2]; Sabine Attinger[3]; Thomas Nagel[4]

[1] *Helmholtz Centre for Environmental Research –UFZ*

[2] *Helmholtz Centre for Environmental Research UFZ / TU Dresden*

[3] *UFZ*

[4] *Technische Universität Bergakademie Freiberg*

Corresponding Authors: thomas.nagel@ifgt.tu-freiberg.de, joerg.buchwald@ufz.de, olaf.kolditz@ufz.de

In the performance assessment of nuclear waste disposal concepts, a thorough analysis of uncertainty and sensitivity of the underlying processes is necessary. In our contribution, we show the applicability of (DoE)-based history matching, a method commonly applied in the oil and gas industry in the context of reservoir modeling, for probabilistic integrity analysis of radioactive waste disposals. The origins of uncertainties of the underlying coupled thermo-hydro-mechanical-(chemical) (THM/C) processes in clay are manifold. One major challenge thereby is, both conceptually and computationally, that the model spans over many spatial and temporal scales. While we typically distinguish between parameter and model uncertainties, both are mostly of the epistemic type. The significant advantages of the applied workflow for uncertainty quantification are its limited technical complexity, its power in dealing with large uncertainties, and its ability to study both parameter and model uncertainties. In our presentation, we show that the workflow is relatively insensitive to specific parameter distribution functions, making it particularly interesting for dealing with epistemic uncertainties in potential nuclear waste disposal sites.
*DoE –Design of Experiment

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Measuring and Modelling Supercritical Adsorption in Shales

Author: Humera Ansari[None]

Co-authors: Martin Trusler [1]; Geoffrey Maitland [1]; Claudio Delle Piane [2]; Ronny Pini [1]

[1] *Imperial College London*
[2] *CSIRO Energy*

Corresponding Author: hsa210@ic.ac.uk

Recent progress in extraction techniques has propelled shale gas production; however, these processes remain largely inefficient. This stems from the lack of understanding of the effect of confinement on the fluids in the shale formations, which have nanometric pores, very low permeability and porosity. While primary methods of recovery provide suitable initial production rates, enhanced means of recovery using CO2 injection 1 may be required to sustain them.

In shale, natural gas is held freely in pores and fractures as well as adsorbed within the micropores of the organic matter 2 and clay minerals. As such, gas adsorption can be used to provide estimates for the Gas-In-Place (GIP) at subsurface conditions, but also serve as a tool for material characterisation by providing insights into the complex pore structure of shale. This investigation aims at (i) quantifying gas adsorption within shale, (ii) resolving the contribution of both the organic matter and clay to gas storage, and the effect of thermal maturity, and (iii) assessing the pore space properties of shale.

CO2 and CH4 adsorption isotherms have been measured using a Rubotherm Magnetic Suspension Balance over a wide range of conditions, i.e. temperatures in the range 283-353K and in the pressure range of 0-300 bar. Two distinct sets of samples have been studied: (i) shales from the Bowland formation in the UK, the Marcellus reservoir in the USA, and the Longmaxi formation in China, as well as (ii) synthetic materials, including mesoporous zeolite and mesoporous carbon. These can serve as analogues for the structure of shale and the organic matter in shale, respectively. We observe that the organic content of the shale can be used to scale adsorption isotherms measured on the mesoporous carbon, thus confirming that (i) shales are largely mesoporous and that (ii) organics play a major role in driving adsorption in shale. However, the presence of microporosity, which is largely associated with clay minerals, is clearly manifested in the isotherm shape and confirmed by comparing observations on shale and mesoporous zeolite. Additionally, the higher thermal maturity of the Marcellus shale which leads to more microporosity in the organic matter, causes a significant increase in adsorption capacities. We have measured a substantial adsorption selectivity of shale towards CO2 as compared to CH4, thus providing an opportunity to exploit the adsorption/desorption process to further enhance gas production and store CO2. The materials have also been characterised using a combination of cryogenic low-pressure (<1 bar) physisorption methods including N2 at 77K, CO2 at 273K and 298K and Ar at 87K.

The supercritical adsorption results have been successfully described using a Lattice Density Functional Theory (LDFT) model, which is extended to the cylindrical pore geometry in this work. The model is able to provide unique insight into the pore-scale interaction between shale and supercritical fluids, by distinguishing between an organic or a clay surface. The model also has predictive capability, which is a significant deviation from empirical approaches such as the Langmuir or BET models 3.

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1017

Effective parameter identification via NMR experiment and simulation using multi-task Bayesian optimization

Authors: Rupeng Li[1]; Igor Shikhov[1]; Christoph Arns[1]

[1] *University of New South Wales*

Corresponding Authors: c.arns@unsw.edu.au, igor.shikhov@unsw.edu.au, rupeng.li@student.unsw.edu.au

Introduction: The petrophysical interpretation of NMR relaxation responses can be enhanced by extracting phase specific physical properties such as surface relaxivity, effective bulk relaxation time, effective diffusion coefficient, susceptibility, etc. Aided by NMR simulation using random walks on micro-CT images, those parameters can be deduced when both producing the same relaxation time distribution. It has been demonstrated that such computationally expensive parameter-searching problems can be solved using Bayesian optimization which proved to be far more superior to grid search or manual search 1. When performing search on similar rocks, such as 2 species of Bentheimer sandstone, it may not be necessary to re-investigate similar settings of parameters as little information is gained. We investigate how to transfer the knowledge between similar tasks to co-optimize the expensive objective functions.

The Optimization Framework: In previous work, we proposed an informed search strategy to identify those properties by minimizing the sum of squared residual (SSR) between the T_2 distribution inverted from NMR simulation and measurement using Bayesian optimization (BO) framework on Gaussian processes (GP). In multi-task Bayesian optimization, GP is extended to multi-task GP with vector-valued output, correlated by a covariance function across tasks K_t whose hyper-parameters are inferred using Markov Chain Monte Carlo (MCMC), similar to how hyper-parameters of covariance function across inputs K_x in single task BO are inferred 2.

Implementation: 4 Bentheimer sandstones, comprising 2 yellow and 2 grey with high similarity within species and moderate similarity across species, are prepared for CT imaging and NMR T_2 measurement. Given the T_2 decays, measured at freq=2MHz, TE=200 and SNR around 300, as well as the corresponding T_2 distributions inverted using active-set method 2, 3 unknown physical parameters, i.e. surface relaxivity of quartz, surface bulk relaxation time of clay and effective diffusion coefficients of clay are of interest. We compared the parameter deduced from Multi-task BO against those from the standard BO and studied the efficiency gained across tasks with variable similarity:

Tasks	Sample A	Sample B
:- – :	:——:	——-:
Tasks 1	BHY1	BHY2
Tasks 2	BHG1	BHG2
Tasks 3	BHY1	BHG1

Results & Conclusion: The cost of optimizing Task 1 & 2 independently using the multi-task BO is almost half of the cost of the standard BO, and in Task 3 the ratio is around 70%. Similar as BO, apart from the statistically optimum solution, multi-task BO also provides solutions which are less optimum in statistics but might be physically more practical. Such solutions form apparent correlation lines or correlation surfaces which help to enhance the interpretation of interplay among physical properties. In conclusion, when searching for good pairs of physical properties of 2 similar rock samples, the multi-task BO can substantially reduce the time required compared with independently optimizing using standard BO. Moreover, simulation is becoming more powerful than before as interpretation of NMR response via simulation becomes progressively cheaper and informative aided by multi-task BO.

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Parametric study on the residual CO2 trapping in Deccan Volcanic Basalt

Authors: Pradeep Reddy Punnam[None]; Shakti Raj Singh Bawal[None]; Himavarsha Pakala[None]; Vikranth Kumar Surasani[1]

[1] *BIrla Institute of Technology and Science*

Corresponding Authors: surasani@hyderabad.bits-pilani.ac.in, p20180042@hyderabad.bits-pilani.ac.in, h20181010024@hyderabad.b
pilani.ac.in

In India, the Deccan Volcanic Provinces predominantly consist of basalt formation layers, which are considered as desirable sites for implementing CO2 sequestration 1. In CO2 sequestration process, after supercritical CO2 (ScCO2) is injected into a geological formation, it undergoes various trapping mechanisms, due to which ScCO2 get safely sealed in the subsurface layer 2. Among various trapping mechanisms, the residual trapping is one of the prominent trapping mechanisms that occurs in the Carbon sequestration process. When the ScCO2 is injected into a geological formation, due to effects of buoyancy, the ScCO2 tends to move upwards and percolate through porous structure. During this time, some amount of ScCO2 gets confined inside the pore space of formation rocks, and some amount ScCO2 gets left behind in the migration pathway. This CO2 can be quantified as residual trapped CO2 3.
The objective of this paper is to conduct a study on residual trapping mechanisms during CO2 sequestration process in the Deccan basalt formation layer. The study on the residual trapping is important as it influences the trapping efficiency of the other trapping mechanisms. This analysis is performed by considering various parameters that effect the efficiency of residual trapping mechanism. The parametric study is conducted on varying petrophysical properties and, at different injection points of geological modelled domain and with the variable injection rates of ScCO2. These simulation studies are analysed over geological time scale. To perform this simulation study, the MRST (MATLAB Reservoir Simulation Toolbox) software is taken into consideration.
MRST uses conservation of mass and modified Darcy's law, which is based on the concept of relative permeability to characterize the flow in the reservoir domain [4]. In MRST, first, the geographical reservoir structure is modelled. Then the petrophysical properties of the domain are induced in the modelled reservoir domain. At the selected injection point, the injection is carried out up to a certain year with a fixed amount of injection rate. Then the movement of CO2 during upward migration and lateral spreading is carefully studied and analysed. The saturation and concentration data of CO2 of each cell below the top boundary are categorized as residual trapping and the cell data in the top grid cell are quantified as structural trapping 5.
The parametric analysis is carried out by analysing the residual trapping percentage at different injection points with fixed injection rate so that the optimal injection point for CO2 sequestration is evaluated. In the second parametric study, the injection rates of CO2 are changed at fixed petrophysical properties and injection point. In varying petrophysical properties study the injection rate and injection point are fixed. These analyses are carried for over a geological time scale, which will help to analyze the dependencies of residual trapping on the surface topography and injection rate. The results provide insights into selection of the suitable petrophysical properties, and optimal injection points with desire injection rate for the safe and efficient implementation of CO2 sequestration, these simulation analyses carried out based on the residual trapping occurrences.

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1020

X-ray CT core flooding study to understand the impact of clay interlayers on supercritical CO2 migration in sandstones

Authors: Liang Xu[1]; Matthew Myers[2]; Cameron White[2]; Qi Li[3]

[1] *University of Chinese Academy of Sciences*

[2] *CSIRO Energy, Australian Resources Research Centre*

[3] *IRSM-CAS*

Corresponding Authors: qli@whrsm.ac.cn, matt.myers@csiro.au, cameron.white@csiro.au, 1921212637@qq.com

The existence of a thin clay interlayer (which has significantly lower permeability/porosity relative to the rest of the formation) in a sandstone formation has a significant influence on supercritical carbon dioxide migration. This will affect the storage characteristics of the target reservoir. Core flooding experiment is the most suitable method to understand the behavior of supercritical carbon dioxide inside the core. A special sandstone is chosen to conduct the carbon dioxide core flooding experiment where are there are two clay interlayers developed inside the core. One is the main clay interlayer whose extension direction is 15 degrees from the flooding direction, and another is a secondary clay interlayer whose extension direction is nearly parallel to the flooding direction. A high-resolution medical X-ray computed Tomography (X-CT) scanner was used to monitor the whole core flooding experiment. Micro-CT imaging was applied to get the porosity and permeability of the both sandstone and interlayer in pore-scale due to the lower resolution of the medical X-CT scanner is in core scale. Using CMG, a core model was constructed and the behavior of supercritical carbon dioxide during drainage process was simulated. The results show that the clay interlayer has the function of both diversion and a barrier during the drainage process. The relationship between flooding direction and clay interlayers have a non-negligible effect on the migration characteristics of supercritical carbon dioxide in anisotropic rocks. When the supercritical carbon dioxide injection direction is opposite to the acute angular opening of the intersecting clay interlayer, supercritical carbon dioxide will accumulate in this semi-closed triangle. However, there is almost no supercritical carbon dioxide in this semi-enclosed area when the injection direction is reversed. Comparing the experiment and simulation results, the differences in pore structure, wettability and miscibility between numerical model and real rock sample are possible reasons that lead to this difference.

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2D to 3D Transform: Material Properties from 2D Images

Authors: Juan Pablo Daza[1]; Amos Nur[1]; Tapan Mukerji[1]

[1] *Stanford University*

Corresponding Author: jpdaza@stanford.edu

Recent advances in 3D imaging allow us to get high resolution geometry of different porous media. However, 3D imaging is expensive and time consuming compared with 2D imaging. 2D imaging gives us high resolution and quality, quickly and with little economical investment.
In this work we propose a geometrical transformation of thin slices to a 3D volume. This transformation is unique, isotropic, analytical, and given that we obtain a 3D volume with the same geometrical characteristics as the 2D image, it enables us to compute physical properties such as permeability, bulk modulus, and conductivity.

We rely completely in the geometrical information available in 2D images, and use this information to construct a 3D volume that preserves the geometrical measurements in 2D. The result is a 3D volume that has the same porosity as the 2D image, as well as a pore-space, well connected and geometrically isomorphic to the pore space of the original sample.

We test the success of this 2D to 3D transform in its ability to predict the physical properties of the sample, in our case the bulk and shear modulus, conductivity and permeability. Obtaining and excellent match of properties computed in volumes obtained from micro-CT, and those properties obtained just from 2D thin slices. For instance in the figure we can see permeability estimates just from a 2D image, compared with the permeability estimates obtained from the original 3D CT-scan, for REV samples the results from 2D images are comparable to those from 3D images.

In conclusion, we have created a transform that creates a 3D volume from a 2D image, with the same geometrical characteristics, reproducing space connectivity, and providing reliable estimates of properties as permeability using only one thin section.

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Simulating Diagenesis: Computing Temporal Pore Structure and Physical Properties Changes Due to Dissolution/Precipitation Under Stress and Reactive Fluid Flow

Authors: Juan Pablo Daza[1]; Tapan Mukerji[1]; Amos Nur[1]

[1] *Stanford University*

Corresponding Author: jpdaza@stanford.edu

Understanding thermo-chemo-mechanical processes with fluids in porous media and rocks is important. Because of the likelihood of fluid-rock chemical interactions, and our limited ability to decipher the mechanical, and fluid flow effects of these coupled processes. One of the missing links is understanding the evolution of elastic and transport properties together with reactive transport. Because the properties of porous media evolve as a result of chemical reactions and vice versa. Capturing this coupling experimentally and theoretically is one of the missing elements in the existing literature. We describe here recent advances in theoretical modeling and simulation of reactive fluids

processes in rocks with complex pore structure, in order to understand the effects of dissolution-induced changes on acoustic velocity, porosity, permeability and electrical properties.

To deal with the problem of modeling the effects of reactive fluids in porous media properties, we adopt the approach by Osher and Sethian (1988) - a conceptual framework for using level sets as a tool for numerical analysis of surfaces and shapes - together with 2D and 3D scanned and segmented pore structure images. The advantage of the level-set approach is that one can perform numerical computations involving complex curves and irregular surfaces on a fixed Cartesian grid without having to parameterize these objects. With this we have already shown how material evolution problems can be mathematically/computationally solved accurately, efficiently (fast), while honoring the coupling between physics and chemistry.

We can get different versions of the pore geometry by using the Osher's approach with the simplest velocity field to change the pore-space interface. Properties such as permeability are then calculated using the Lattice-Boltzmann method (Keehm, Mukerji, and Nur 2001), for each change in the geometry. The results of the calculated permeability are compared with the experimental observations (Bourbié 1985) for Fountainebleau sandstone. Thus the method used in our work is the enabling technology to model and simulate the structural changes of the different components of the porous media, under different physical and chemical processes.

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Transfer of mass and momentum at interface between porous media and free flows

Authors: Shervin Bagheri[1]; Ugis Lacis[1]; Simon Pasche[1]; Yogaraj Sudhakar[2]

[1] *KTH*

[2] *KTH*

Corresponding Author: shervin@mech.kth.se

Porous materials play a critical role in transport phenomena. We characterize porous materials by their ability to exchange mass and momentum with free-flowing fluids. We derive a homogenized macroscopic model for fluid flows over-ordered homogeneous porous surfaces. The unconfined free-flow is described by the Navier-Stokes equation, and the Darcy equation governs the seepage flow within the porous domain. Boundary conditions that accurately capture mass and momentum transport at the contact surface between these two domains are derived using the multiscale homogenization technique. In addition to obtaining the generalized version of the widely used Beavers-Joseph slip condition for tangential velocities, the present work provides an accurate formulation for the transpiration velocity and pressure jump at fluid-porous interfaces; these two conditions are essential for handling two- and three-dimensional flows over porous media.

All the constitutive parameters appearing in the interface conditions are computed by solving a set of Stokes problems on a much smaller computational domain, making the formulations free of empirical parameters. The tensorial form of the proposed interface conditions makes it possible to handle flows over isotropic, orthotropic, and anisotropic media.

The accuracy of the proposed macroscopic model is numerically quantified for flows over porous and rough walls by comparing the results from our homogenized model with those obtained from geometry-resolved microscopic simulations. We validate and demonstrate the physical significance of the effective conditions on two canonical problems – a lid-driven cavity and turbulent channel flow, both with non-smooth bottom surfaces.

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Contact line motion: comparing molecular dynamics, the phase field model and the sharp interface model.

Authors: Ugis Lacis[1]; Petter Johansson[2]; Thomas Fullana[3]; Stéphane Zaleski[4]; Berk Hess[2]; Gustav Amberg[5]; Shervin Bagheri[1]

[1] *Department of Mechanics, KTH, Sweden*

[2] *Department of Applied Physics, KTH, Sweden*

[3] *Sorbonne Université and CNRS, France*

[4] *Institut Jean Le Rond d'Alembert*

[5] *Department of Mechanics, KTH & Södertörn University, Sweden*

Corresponding Authors: shervin@mech.kth.se, hess@kth.se, pettjoha@kth.se, stephane.zaleski@gmail.com, ugis@mech.kth.se, tomasfullana@gmail.com, gustav.amberg@sh.se

Motion of the contact line is ubiquitous in both nature and engineering. For example, imbibition or drainage process of a liquid in a porous material involves a large amount of contact lines, continuously moving over the material pores. The classical no-slip condition results in infinitely large stresses and always static contact line, which is incompatible with everyday observations. A popular resolution of this paradox is a Navier-slip boundary condition for the tangential fluid velocity on the solid surface, set by a slip length ℓ_s. However, realistic molecular models of water on a glass-like surface (consisting of SiO_2 molecules) show practically no-slip between the first water layer and the surface. We set-up simple Couette flow between two plates, with a water droplet sheared in the middle of the domain. We carry out molecular dynamics (MD) simulations using GROMACS code of the selected configuration to obtain a reference data. We then evaluate two continuum models –diffusion based Cahn-Hilliard phase field (PF) model and a sharp interface Volume of Fluid (VOF) model –against the MD results. We assess the accuracy of both continuum models by looking at steady state interface profile, drop displacement and flow field. In particular, we evaluate the importance of the Generalized Navier Boundary Condition (GNBC) –proposed recently to improve the physical model near the moving contact line –for accurate representation of the reference results. The findings of our research will serve as a stepping stone towards accurate and efficient modelling of many important problems containing contact line motion, such as imbibition or drainage in porous media.

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Experimental study of contaminant transport in coupled fracture-porous medium systems

Author: Monika S. Walczak[1]

Co-authors: Hamidreza Erfani Gahrooei [1]; Nikolaos Karadimitriou [2]; Ioannis Zarikos [3]; S. Majid Hassanizadeh [4]; Vahid.J Niasar

[1] *University of Manchester*

[2] *Institute of Mechanics (CE), Stuttgart University*

[3] *Eindhoven University of Technology*

[4] *Utrecht University*

Corresponding Authors: vahid.niasar@manchester.ac.uk, monika.walczak@manchester.ac.uk, nikos.karadimitriou@mechbau.uni-stuttgart.de, hamidreza.erfanigahrooei@postgrad.manchester.ac.uk, i.zarikos@tue.nl

The transport of contaminants in fractures coupled with porous media is not a straight forward process to predict and model, due to the large contrast between the time scales in the two domains.
This research aims at investigating the conditions at the interface between the two domains, the mass exchange rate between them, and the evolution of dispersion in the porous medium under steady-state, single flow conditions.
Water-based ink, acting as the contaminant, is introduced into a fracture coupled with a porous medium in an artificial, fully saturated with water, Poly-Di-Methyl-Siloxane (PDMS) micromodel. We call this process as contamination. This process, and the subsequent clean-up, when the micromodel is flushed with clean water, were carried out for three injection rates of 0.01, 0.1 and 1 ml/h. By employing image processing to the acquired images from both processes, we investigate the hydrodynamic interface conditions, the mass exchange rate between the fracture and the porous medium, and the induced dispersion in the porous medium.
In contrast to most of the existing theoretical and numerical works in the literature, we found that the mass exchange rate coefficient is not constant, but it varies significantly. It also shows a significant difference in its value depending on the process (contamination or clean-up). These findings are in contradiction to the established understanding of a linear and unique, non-equilibrium mass exchange between the fracture and the matrix. We also observed that counter-diffusion during clean-up is slowing down the whole process, in comparison to contamination.
The results of this research shed new light into one of the potential reasons for very long time required to cleanup contamination from the matrix.

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Experimental investigation of low salinity water flooding efficiency in tight carbonate fractured oil reservoirs; a case study

Authors: Rasoul Mokhtari[1]; Mohammad Sadegh Mousapour[2]; Pourya Malmir[3]; Amin Alinejad [4]; Shahab Ayatollahi[4]

[1] *The Danish Hydrocarbon Research and Technology Centre*

[2] *Sahand University of Technology (SUT), Tabriz, Iran*

[3] *Petroleum University of Technology (PUT), Ahwaz, Iran*

[4] *Sharif Upstream Petroleum Research Institute (SUPRI), Sharif University of Technology, Tehran, Iran*

Corresponding Authors: mousapour.sadegh@gmail.com, rasoulm@dtu.dk, shahab@sharif.ir, malmir.pourya@gmail.com, sir.alinejad@gmail.com

Effectiveness of waterflooding in fractured oil reservoirs critically depends on imbibition of water from fracture network into the oil-saturated matrix, which is governed by the capillary forces, and is related to the rock wetting state. Since imbibition mechanism is the main oil production mechanism in tight fractured reservoirs, in which high amount of oil is trapped in water-invaded zone, this paper evaluates the effect of brine salinity on oil recovery through a series of imbibition experiments. Before that, by means of conducting contact angle measurements over a period of 540 hours, wettability alteration indices were identified. To have a better insight, the initial and final pH values of brines used in these experiments are measured. In addition, the Equilibrium Interfacial Tension

(EIFT) values for different brines and crude oil are measured. Therefore, the main objective of the current research work is to evaluate the effectiveness of low salinity water flooding on imbibition enhancement in an Iranian tight carbonate (mostly calcite) reservoir. In addition, this research aims to correlate wettability alteration indices with oil recovery factor during imbibition process. Meanwhile the wettability alteration mechanisms are investigated as well.
Contact angle measurements illustrate that low salinity water cannot change the calcite wettability state from completely oil-wet to completely water-wet state. Highest wettability alteration index (WAI) was observed for two-time diluted seawater compared to other dilutions of seawater, in which the final contact angle was approximately 100 degree. Comparing the initial and final pH values before and after contact angle measurements for different brines shows that calcite dissolution increases as the brine salinity decreases. On the other hand, IFT measurements results showed a declining trend by decreasing the brine salinity. However, dynamic IFT measurements revealed that five-time diluted seawater has the highest rate of change of IFT value. The imbibition mechanism is the result of capillary and gravity forces. Therefore, rate of imbibition is dependent to both IFT and wettability state, simultaneously. The imbibition production curves illustrated that initial recovery is governed with IFT values and the ultimate recovery factor is controlled with WAI. The dimensionless inverse bond number could relate IFT values and WAI to recovery factor, sufficiently. This study shows that, although low salinity water could not completely alter the wettability state of calcite, it still is able to improve oil recovery through imbibition enhancement. The other important outcome is finding a practical way to combine both rock-fluids (wettability) and fluid-fluid (IFT) interactions and predict the recovery factor in an imbibition process. It really helps to have a clear insight into screening the best injecting fluid even without conducting time consuming experiments.

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Dynamic Pore-Scale Dissolution by CO2-Saturated Brine in Carbonates: Impact of Homogeneous versus Fractured versus Vuggy Pore Structure

Authors: Yingwen Li[None]; Yongfei Yang[1]

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

Corresponding Authors: yangyongfei@upc.edu.cn, 1047971053@qq.com

The initial pore structure of limestone has an important influence on the dissolution pattern, which in turn affects the safety of carbon capture and storage. We studied the effect of initial pore structure on the dissolution pattern in limestone and selected three typical carbonate rocks, which ranged in their heterogeneity, i.e. a homogeneous sample A, a fractured sample B and a vuggy sample C. CO2 saturated brine was injected into these samples and the samples were imaged periodically by X-ray micro-tomography. For the homogeneous sample A, the preferential channel was surrounded by branched channels. The original fractures became the main flow path in fractured sample B. However, only one dominant channel existed in the vuggy sample C, which results in a sharp increase in permeability. The Damköhler number of the homogeneous sample is lower than that of the other two samples, representing uniform dissolution. However, this uniform dissolution pattern transforms to a single preferential channel growth after injecting sufficient reactive fluid. Moreover, we believe that the research scale has a significant effect on the Da distribution range of uniform or non-uniform dissolution pattern. With the decrease of research scale, dissolution tends to be non-uniform. Overall, we visualized and quantified three typical dissolution patterns of carbonate rocks at micron scale, which have obvious characteristics both in spatial morphology and in parametric variation. Our work implies that more attention should be paid to reactivation of geological faults and damage around wellbore when CO2 is injected into fractured-vuggy carbonate reservoirs.

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An improved empirical model considering viscous coupling effect for hydraulic conductance of three-phase flow in pore network modeling

Author: Fei Jiang[1]

Co-authors: Jianhui Yang [2]; Edo Boek [3]; Takeshi Tsuji [4]

[1] *Faculty of Engineering, Yamaguchi University*

[2] *GRC, TOTAL*

[3] *Queen Mary University of London*

[4] *Kyushu University*

Corresponding Authors: e.boek@qmul.ac.uk, jianhui.yang@total.com, fjiang@yamaguchi-u.ac.jp

The momentum transfer across fluid interfaces in multi-phase flow leads to an unneglectable viscous coupling effect. In this study, we use the lattice Boltzmann method (LBM) as a direct simulator to solve the three-phase flow at pore scale. The accuracy of the multiphase LBM solver to capture viscous coupling effect is validated by performing the benchmark three-phase co-current flow between two parallel plates. The viscous coupling effects are then investigated for various fluid configurations in simple pore geometries with different conditions in terms of saturation, wettability and viscosity ratio. It is found that the viscous coupling effect strongly depends on the viscous ratios, while is less sensitive to saturation or wettability. A parametric model is then proposed to estimate the viscous coupling effect as a function of viscosity ratios. Moreover, an elegant approach using machine learning is proposed to predict the multi-phase conductance by a trained Artificial Neural Network (ANN) from the direct simulation database. These empirical models are very practical and can be easily incorporated into existing pore network model to eliminate errors from viscous coupling effect. The data-driven approach can be extended to developing more sophisticated pore network models containing more pore-scale mechanisms.

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Gas separation in bent microchannel at low Reynolds number

Authors: Minh Tuan Ho[1]; Jun Li[2]; Wei Su[1]; Lei Wu[3]; Matthew Borg[4]; Zhihui Li[5]; Yonghao Zhang[1]

[1] *University of Strathclyde*

[2] *King Fahd University of Petroleum and Minerals*

[3] *Southern University of Science and Technology*

[4] *University of Edinburgh*

[5] *China Aerodynamics Research and Development Center*

Corresponding Authors: wul@sustech.edu.cn, wei.su@strath.ac.uk, minhtuanho.vn@gmail.com, matthew.borg@ed.ac.uk, zhli0097@x263.net, junli@kfupm.edu.sa, yonghao.zhang@strath.ac.uk

Flow characteristics in microchannels have been studied extensively because of their wide applications in MEMS devices and tight porous media. However, flow separation, a fundamental phenomenon, in bent microchannel has attracted much less attention compared to that in macrosystem, as the Reynolds number (Re) is usually small. Nevertheless, in microchannel the Knudsen number (Kn), which is defined as the ratio between the mean free path of gas molecules and the characteristic flow length, is not small; and this may introduce new flow physics which does not occur in macrosystems.

Based on the numerical solution of the gas kinetic equation in well-resolved spatial grids, the separation of rarefied gas flow in a microchannel with double rectangular bends connecting two reservoirs is investigated over a wide range of Kn (10^{-4} to 10) and Re (10^{-7} to 40), see Figure 1(a). The velocity slip at the channel surface, which is one of the major rarefaction effects when Kn is small, is found to be responsible for "late-onset"and "early-onset"(in term of Re) of flow separation at the concave and convex corners, respectively. Flow separation is observed for Kn up to 0.04 while the adverse pressure gradient occurs in bent region for all examined Kn. Due to the secondary flow and adverse pressure gradient near the rectangular bends, the mass-flow rate ratio between the bent and straight channels of the same length is a non-monotonic function of the Knudsen number, see Figure 1(b). Compared to the straight channel of the same length, the bent channel may yield higher mass flow rate from the continuum regime to the early transitional regime, thanks to a significant reduction of friction loss on the concave walls.

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Role of Connate Water in Immiscible Viscous Fingering

Authors: Lucas Mejia[None]; Matthew Balhoff[1]; Kishore Mohanty[2]

[1] *University of Texas at Austin*

[2] *The University of Texas at Austin*

Corresponding Authors: lmkerguelen@utexas.edu, balhoff@mail.utexas.edu, mohanty@mail.utexas.edu

Understanding multiphase displacements in porous media is important for many subsurface applications such as enhanced oil recovery, CO2 sequestration, and removal of non-aqueous phase liquid contaminants. Multiphase displacements in the subsurface are understood to be stable if the injection rate is small and the mobility ratio is favorable (the injected phase is less mobile than the resident phase). In the context of geoengineering, the former condition is usually met as most subsurface processes involve small flow rates, while the latter condition can be met by adjusting the viscosity of the injected fluid. If the injected fluid is viscous enough and can be injected without breaking the rock, the displacement should be piston-like. This work is novel because we show that pre-wetting residual water films can promote viscous fingering even when a very viscous fluid (glycerol solution with viscosity 51cp) displaces a much less viscous oil (viscosity 13cp) at a small injection rate (Ca<10-5).
To show that residual water films can promote viscous fingering at favorable viscosity ratios, we

conducted microfluidic experiments in a novel platform that we introduced previously (Mejia et al., 2020). The micromodel is 40cm long, in the length scale of a rock core, has a heterogeneous pore structure, and includes shallow pore throats. We saturated the chip with viscous glycerol (51cp), then displaced the viscous glycerol solution with oil (13 cp) until no more glycerol could be removed. Then, we injected glycerol solution (51cp) at a small flow rate (5μL/hr). This displacement was stable. Moreover, we conducted an analogous experiment where the micromodel was initially saturated with deionized (DI) water (1cp). Then, oil (13cp) displaced the resident DI water until no more water could be removed. Finally, viscous glycerol (51cp) was injected at a small flow rate (5μL/hr) to displace the oil. This displacement was unstable.
We found that the viscosity of the residual water results in a marked difference in displacement efficiency even though the injected glycerol solution was equally viscous, and the residual water content was similar for both cases (<5% by volume). The first case, where the residual water was 51cp, did not show fingering. In the second case, where the residual water was 1cp, the glycerol solution fingered through the oil, which resulted in smaller oil recovery at the same pore volumes injected. The fingering is surprising as the viscosity ratio is very favorable in both cases. Additionally, while the first case was stable, the second case is more commonly encountered in subsurface applications such as polymer flooding, where the resident fluid is brine and the injected fluid is viscous polymer solution .

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UNCERTAINTY QUANTIFICATION IN A MODEL FOR FOAM FLOODING IN POROUS MEDIA

Author: Rodrigo Weber dos Santos[1]

Co-authors: Andrés R. Valdez [1]; Bernardo Martins Rocha [1]; Grigori Chapiro [1]

[1] *Universidade Federal de Juiz de Fora*

Corresponding Authors: rodrigo.weber@ufjf.edu.br, grigorichapiro@gmail.com, bernardomartinsrocha@ice.ufjf.br, arvaldez@ice.ufjf.br

Computational models and numerical simulators have demonstrated to be extremely relevant to predict the efficiency of different enhanced oil recovery (EOR) techniques. In particular, we focus on foam flooding cases, where the use of foam alters the mobility of gas, avoiding the phenomenon of fingering. In most cases, foam flooding models have parameters that are hard to determine due to technical limitations or measuring errors. In such cases, the outputs of the simulations contain a level of uncertainty that needs to be assessed to check the reliability of the response for forecasting and decision-making purposes. In this work, we have adopted the linear kinetic foam flooding model proposed by Ashoori et al. 1. Uncertainty quantification and sensitivity analysis studies were performed considering relevant quantities of interest. The methods used to propagate uncertainties from the input parameters to the model's output were accelerated by emulators based on polynomial chaos expansion (PCE). In addition, the probability distributions of the input parameters were estimated using the Markov Chain Monte Carlo (MCMC) method. This study allowed us to determine how the output quantities are affected by uncertainties in the input parameters, and also the parameters that have the most significant impact on the outputs.

Acknowledgements: This research was carried out in association with the ongoing R&D project registered as ANP 20715-9, "Modelagem matemática e computacional de injecão de espuma usada em recuperacão avancada de petróleo"(Universidade Federal de Juiz de Fora (UFJF) / Shell Brasil / ANP) Mathematical and computational modeling of foam injection as an enhanced oil recovery technique applied to Brazil pre-salt reservoirs, sponsored by Shell Brasil under the ANP R&D levy as "Compromisso de Investimentos com Pesquisa e Desenvolvimento". This project is carried out in partnership with Petrobras.

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Modeling perfusion in cardiac tissue

Author: Rodrigo Weber dos Santos[1]

Co-authors: João R. Alves [1]; Evandro D. Gaio [1]; Rafael AB de Queiroz [1]

[1] *Universidade Federal de Juiz de Fora*

Corresponding Authors: bonfimraf@gmail.com, rodrigo.weber@ufjf.edu.br, joaorafaelalves@hotmail.com, evandrodgaio@gmail.com

This work presents a mathematical model to describe the dynamics of perfusion in cardiac tissue. The new model extends a previous one 1 and can be used in the quantification of clinical information usually obtained via imaging techniques, such as cardiac magnetic resonance imaging (MRI) and computed tomography (CT) perfusion exams.
The new model treats the extravascular domain as a continuum porous medium, whereas the arterial trees are explicitly represented by graphs or a collection of one-dimensional tubes that bifurcate.
Poiseuille's law is used to obtain pressure and velocity in the arterial trees. For the extravascular domain, Darcy's law is adopted.
We propose new reaction-diffusion-advection equations to capture the dynamics of contrast agents that are typically used in CT or MRI perfusion exams.
Different scenarios were simulated and compared to clinical images: normal perfusion; endocardial ischemia due to stenosis; and myocardial infarct. The computational model was able to correlate anatomical features, stenosis and the presence of fibrosis, with functional ones, cardiac perfusion. Altogether, the results obtained suggest that the models can support the process of non-invasive cardiac perfusion quantification.

1 Simulation of the Perfusion of Contrast Agent Used in Cardiac Magnetic Resonance: A Step Toward Non-invasive Cardiac Perfusion Quantification. JR Alves, RAB de Queiroz, M Bär, RW dos Santos. Frontiers in Physiology 10. 2019

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Integrating geological data and upscaling static and dynamic properties for a CCS project.

Authors: Mark Knackstedt[1]; Mohammad Saadatfar[2]; Robert Sok[3]; Paal Eric Oeren[4]; Lachlan Deakin[3]

[1] *Prof*

[2] *Australian National University (ANU)*

[3] *ANU*

[4] *Petricore*

Corresponding Authors: l.deakin@anu.edu.au, paal.eric.oeren@petricore.com, robert.sok@anu.edu.au, mark.knackstedt@anu.edu.au, mohammad.saadatfar@anu.edu.au

Carbon capture and sequestration (CCS) offers an approach for permanent storage of carbon in geological formations. This presentation will describe a research program which supports the Surat basin CCS pilot project. The Surat CCS storage project requires accurate predictions of the extent of plume movement within the storage complex. The aim of the project is to quantify the uncertainty in the predictions of the lateral extent and impact of the injected GHG stream. Small-scale geological features and heterogeneities have a significant impact on the plume movement in the subsurface but cannot be directly incorporated into field scale simulation models because of limitations in computer speed. The average effects of small scale heterogeneities must be accounted for via an integrated multiscale workflow. A multiscale imaging and analysis workflow is described here.

We present an integrated pore to geo-cell geological description and calibrated static and flow property data from pore to whole core scales on a continuous 50 meters of core from a well at the Surat CCS demonstration (schematic shown in Figure below). The data includes continuous imaging of 50m of whole core scanning at resolutions of 25 microns. This enables one to clearly observe facies changes at the sub-mm scales along continuous lengths of whole core material. This in turn enables one to correlate high resolution image data directly to whole core material and with robust rock typing methods enables one to couple geological and image-based classification/typing. This further enables one to propagate laboratory scale measurements directly to the whole core scale. Porosity and permeability are measured at millimetric intervals and drainage capillary pressure measured for different rock types.

Heterogeneity in permeability is observed at the mm-cm scales in sequences of the Surat core. Many laminations exhibiting significant permeability contrasts at cm scales in sand:silt intervals. Laboratory data and log measurements do not capture the extent of the heterogeneity. We explicitly illustrate the role of varying rock type on the dynamic properties both horizontally and vertically. We illustrate that upscaled data for dynamic properties (Kr,Pc) need not lie within the envelope of the master curves for separate rock types. In forward work we discuss the effects of small scale heterogeneities on the global flow and the resultant quality of the geocell static and dynamic properties within the static/dynamic models. This can impact on the upscaled equivalent flow properties used in the static and dynamic model, and ultimately impact the predictions of global flow and plume movement in the dynamic model.

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Study on formation water mobility and its determination method in tight sandstone gas reservoirs

Author: Dongsheng Li[None]

Co-authors: Yuliang Su [1]; lei li [2]; Xiaogang Gao [1]; Jingang Fu

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

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

Corresponding Authors: gaoxiaogang1@126.com, lei.li@upc.edu.cn, fujingang86@sina.com, lidongsheng_upc@163.com, suyuliang@upc.edu.cn

Tight sandstone gas reservoirs have low porosity, low permeability, and complicated gas-water distribution. The severe formation water production seriously restricts gas well productivity. Accurate expression of formation water mobility is helpful to control water production and increase gas rescovery. At present, the most popular method to determine irreducible water saturation and movable water saturation are NMR and centrifugation method. This paper considers that the mobility of formation water is closely related to the pore structure of rocks. The purpose of this article is to study the relationship between reservoir physical parameters and the mobility of formation water, and to determine the formation water mobility in reservoirs with different physical properties.
In this study, The porosity and permeability of the core were measured using pulse attenuation method. The pore size distribution of the core is measured by NMR. The mineral composition of the sandstone core samples was determined by X-ray experiment. Based on the formation water force analysis in the channels and the occurrence state of formation water in different pore structures, the formation water mobility is studied. A new method of dividing the mobility of formation water by the combination of centrifugal method and NMR is proposed. On this basis, the relationship among porosity, permeability, pore size distribution, rock mineral composition and formation water mobility is established.
The results show that the formation water mobility is dependent on the pore structure. An interesting finding is that there is no absolute limit between movable or immovable formation water. According to the mobility, formation water can be divided into irreducible water, movably irreducible water and movable water. The mineral composition has little effect on the mobility of formation water.
Through the measurement of the pore structure of the corresponding formation rock, the mobility of the formation water can be expressed quantitatively with the known parameters of irreducible water saturation, movably irreducible water saturation. The movable water saturation of the formation can be calculated when the original water saturation is given.. It is of great significance for the development of tight sandstone gas reservoirs and reduction of formation water production.

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Insights into dynamic interfacial tension of oil-brine system in the presence of asphaltene

Authors: Amir Mohammadi[1]; Mohammad Simjoo[2]; Mohammad Chahardowli[2]

[1] *Faculty of Petroleum and Natural Gas Engineering, Sahand University of Technology, Iran*

[2] *Department of Oil and Natural Gas Engineering, Sahand University of Technology, Tabriz, Iran*

Corresponding Authors: chahardowli@sut.ac.ir, am_mohammadi@sut.ac.ir, simjoo@sut.ac.ir

Asphaltene is one of the main polar components of the crude oil that exhibits surface-active property. The effect of asphaltene on the interfacial property of oil/water interface is one of the key important parameters that could affect the performance of water based EOR processes. Few studies highlighted the effect of ionic strength on the interfacial property of the asphaltenic oil, but yet several questions have remained about the dynamic interfacial property of the asphaltene molecules on the oil/brine

interface and its effect on the interfacial tension (IFT). In this paper, the effect of salinity and asphaltene concentration on the IFT of the oil/brine system was investigated by using dynamic interfacial tension measurement. In order to track the surface activity of the asphaltene molecules, the oleic phase was simplified in the form of a miscible mixture of toluene and n-heptane (Heptol) with an asphaltene concentration ranging from 0.1 to 3 wt%. Seawater (SW) and its different salinity (0.1SW and 2SW) were prepared to mimic low and high salinity water conditions. The asphaltene used in this study was extracted from one of the Iranian oil reservoirs. Also, all the IFT measurements were carried out at the ambient conditions.
Results showed that the presence of asphaltene molecules in the brine/Heptol system leads to a meaningful reduction in the IFT profile in all the salinity range. Such IFT reduction gives an impression about the adsorption of asphaltene molecules on the brine/Heptol interface that obeys a Langmuir-type adsorption model. The effect of asphaltene on the IFT profile of the brine/Heptol system was characterized by an initial sharp decay followed by a gradual reduction toward an equilibrium value. As to the experimental data, the dynamic IFT profile for the case of SWbrine/Heptol/0.1wt%asphaltene was as follows: an initial value of 28.5 (±0.3) mN/m followed by a sharp decay to 23.4 mN/m over several seconds and then a gradul reduction toward an equilibrium value of 21.2 mN/m, while in the absence of asphaltene the equilibrium IFT was about 25.3 mN/m. As to the ionic strength, the equilibrium IFT of the brine/Heptol/asphaltene in the presence of SW was lower than that of 0.1SW, but such reduction was not that much pronounced in the presence of 2SW. This could be attributed to the presence of an optimum salinity range to facilitate the migration of asphaltene molecules into the brine/Heptol interface. In all the salinity range, there was a positive impact on the IFT reduction by increasing asphaltene concentration up 0.5wt% such that at SW salinity, IFT diminished from 25.3 to 16.5 mN/m. But, beyond this concentration only a slight reduction in IFT was observed, 16.1 mN/m at 3wt% asphaltene. Such behavior could be reminiscent of the presence of a critical micelle concentration for a surface active material that indicates that the brine/Heptol interface was almost occupied by asphaltene molecules at 0.5wt% concentration.

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Extremely large deformation and fracture of hydrogels

Authors: Jacques Huyghe[1]; Eanna Fennell[1]

[1] *University of Limerick*

Corresponding Authors: jacques.huyghe@ul.ie, eanna.fennell@ul.ie

Ionized hydrogels, as osmoelastic media, swell enormously (1000 times its original volume in unionized water) due to the osmotic pressure difference caused by the presence of the negatively charged ion groups attached to the solid matrix polymer chains). The coupling between the extremely large deformations (induced by swelling) and fluid permeation is a field of application that regular u-p poroelasticity formulations cannot handle. We present a mixed hybrid finite element (MHFE) computational framework featuring a three-field (deformation-chemical potential-flux) formulation. This formulation guarantees that mass conservation is preserved both locally and globally. The constitutive formulation of swelling is composed of an elastic, a mixing and a ionic free energy term. The MHFE model stays robust and accurate for a volume increase of more than 3000%. An associated XFEM formulation for fracture is able to simulate step wise propagation in gels as experimentally observed in earlier studies.

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CO2 Mobility Control by Foam at the Pore Level

Author: Tore Føyen[1]

Co-authors: Malin Haugen [1]; Benyamine Benali [1]; Martin A Fernø [1]

[1] *Department of Physics and Technology University of Bergen*

Corresponding Author: tore.foyen@uib.no

Reduction of the CO2 mobility is beneficial during subsurface sequestration of anthropogenic CO2 in saline aquifers and hydrocarbon reservoirs by mitigating flow instabilities leading to early gas breakthrough and poor sweep efficiency. Foam can be described as discontinued gas phase, separated by a continuous thin liquid film called lamellae and can be utilized as a measure to reduce CO2 mobility as each individual bubble at the pore level will hamper flow.

Pore level fluid configuration and flow phenomena during CO2 foam generation and coalescence are captured across 22mm X 27mm porous micromodels with an irregular pattern based on real rock thin sections at 1-micrometer resolution during CO2 foam injection. The pore space was pre-saturated with an aqueous solution containing a foaming agent and the injection of CO2 resulting in foam generation was imaged as dense time series using a Zeiss Axio Zoom v16 epi-illumination microscope equipped with an automated mechanical scanning stage controlled by the microscope software. The scanning stage gives the ability to capture an extended field of view, proven valuable as the spatial distribution features during foam generation and coalescence in the heterogeneous micromodel was revealed.

Time lapse imaging during dynamic injection tests results in large temporal and spatial data information sets. An automatic, systematic interpretation using computer vision transforms images into meaningful statistics and captures features of interest in the micromodel pore structure. Such data can reveal foam generation mechanisms and be utilized to easily compare experimental variables such as different foam agents, concentrations and boundary conditions.

Foam generation by nucleation of foam bubbles at permeability contrasts and subsequent backward propagation of foam (towards flow direction) was revealed as the dominate foam generation mechanism. The backward propagation of foam is likely caused by increased pressure gradients due to the initial nucleation and the permeability contrast. Generation of flow channels that are not hampered by foam bubbles was observed after several pore volumes

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Effects of Quasi-Saturation on Water Table Dynamics, Estimated Recharge Rates, and Groundwater Modeling

Authors: Roger Gonçalves[1]; Hung K. Chang[1]; Martinus van Genuchten[2]

[1] *São Paulo State University, UNESP*

[2] *Utrecht University*

Corresponding Authors: rvangenuchten@hotmail.com, chang@rc.unesp.br, roger.dias@unesp.br

This study focuses on the presence of a quasi-saturated layer near the water table, defined as the uppermost dynamic portion of the saturated zone subject to water table fluctuations. Entrapped air here may cause substantial reductions in the hydraulic conductivity and fillable pore water (e.g., Faybishenko et al., 1995). Air entrapment is caused by a rising water table, usually as a result of groundwater recharge. The most significant effects of entrapped air are recharge overestimation when based on methods that use specific yield, such as the water table fluctuation method (WTF), and a poor description of the water table dynamics in time. These effects can also impact estimation of flow velocities and contaminant transport rates in groundwater as such. In attempts to better quantify actual groundwater recharge rates and the effects of entrapped air, numerical simulations with the FEFLOW groundwater flow model (Diersch, 2014) were carried out using a quasi-saturated layer. Calculated recharge rates for a pilot area in Rio Claro, Brazil represented 16% of the average precipitation over an 8-year period, approximately half of estimates using the WTF method. Very accurate descriptions could be obtained of the water table fluctuations in time over an 8-year period. Vadose zone recharge rates and water table fluctuations calculated with the one-dimensional Richards equation were relatively close qualitatively, but still deviated noticeably from the observed data. Modified FEFLOW calculations showed that air entrapment amounted to a fillable porosity of 0.07, significant lower that the value of 0.17 obtained experimentally. These and other numerical results showed that entrapped air in the quasi-saturated layer can significantly affect estimates of prevailing water table oscillations, groundwater recharge rates and, more generally, calculated groundwater flow rates. Please note that this presentation is part of an Interpore 2020 Minisymposium honoring Professor Rainer Helmig for his long-time contributions to contaminant hydrogeology, especially in the areas of multiphase flow and multicomponent transport, as well as for his long-time commitment to student education and the porous media profession in general.

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Micro-CT image resolution limitation effects on NMR simulation response

Authors: Yingzhi Cui[1]; Igor Shikhov[1]; Christoph Arns[1]

[1] *UNSW*

Corresponding Authors: igor.shikhov@unsw.edu.au, c.arns@unsw.edu.au, yingzhi.cui@unsw.edu.au

Nuclear magnetic resonance (NMR) is an efficient, non-invasive technology for prediction of petrophysical properties on sedimentary rocks. The transverse relaxation time (T2) is utilized as well-logging parameter to characterize pore size distribution, permeability and fluid typing in the assumption of fast diffusion. However, micro-porosity presents e.g. in clay regions complicates the calculation of transverse relaxation responses due to resolution limitations in micro-CT images. Clay minerals exhibit a wide range of magnetic susceptibility which may lead to a broad distribution of internal gradients, pushing the relaxation regime out of the fast diffusion regime. The purpose of this study is to analyze these clay effects on transverse relaxation by implementing a dual-scale model where the clay micro-structure is resolved explicitly in the simulation on tomographic images.

We reconstruct the 3D clay morphology from 2D SEM images as the fine-scale model. The coarse-scale model is the segmentation of micro CT image. We first obtain the effective properties from the reconstructed clay model directly. By assigning these values into the coarse-scale model and matching with experimental data of T2, the surface relaxivity and magnetic susceptibility for each (effective) phase can be determined. The transverse relaxation rate enhancement due to clay (RREC) is estimated by the control variable method. Secondly, we calculate the 3D relaxation regime distribution by comparing three relevant length scales (diffusion length, dephasing length and structural length) in each voxel to analyze the behavior in the unresolved micro pore space. Finally, the unresolved clay phase in the segmentation is substituted by the reconstructed clay model. We calculate the internal field by dipole approximation in the fully resolved image to analyze internal gradients change from micro to macro pore space.

The results indicate that paramagnetic clay minerals shorten transverse relaxation time significantly. The relaxation behavior in the micro pore is dominated by localization regime rather than fast diffusion even in the low field strength. The internal gradients change in dual-scale pore can be characterized by fully resolved image. The improved modeling capacity may lead to significantly more robust interpretations of NMR response for porous media.

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Complex interplay between wettability and pore geometry controlling dynamics of two phase flow in heterogeneous porous media

Authors: Sahar Bakhshian[1]; Rabbani Harris [2]; seyyed hosseini[3]; Nima Shokri[4]

[1] *Bureau of Economic Geology, University of Texas at Austin*

[2] *Texas A&M University at Qatar*

[3] *The University of Texas at Austin*

[4] *Hamburg University of Technology*

Corresponding Authors: nima.shokri@tuhh.de, sahar.bakhshian@beg.utexas.edu, harris.rabbani@qatar.tamu.edu, seyyed.hosseini@beg.utexas.edu

This study presents the coupled effects of wettability and pore geometry on pore-scale dynamics of immiscible two-phase flow in porous media. Using a multiphase lattice Boltzmann (LB) model, we

perform a pore-scale simulation of two-phase flow in homogeneous and heterogeneous porous samples under strong-, intermediate- and weak-wet conditions. The observed invasion patterns indicate that wettability and pore-space complexity which are ignored commonly in the classical Lenormand phase diagram (Lenormand et al. 1988) play crucial roles in controlling the displacement patterns. Dependence of the recovery efficiency of the defending fluid on the wettability is delineated in both homogeneous and heterogeneous porous media. As the wetting condition changes from strong drainage to imbibition, we observed a transition from burst to corner flow leading to the compact displacement and hence a higher recovery efficiency in the heterogeneous sample.
The present fundamental study sheds new lights on how the rock wettability influences oil/gas displacement efficiency in porous media particularly in applications such as CO2 storage, soil remediation and enhanced oil recovery.

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A True-to-Mechanism Model for Plasma and Transport Phenomena inside a DBD reactor

Authors: Nadia Bali[1]; Christos Aggelopoulos[1]; Eugenios Skouras[2]; Christos Tsakiroglou[1]; Vasilios Burganos[1]

[1] *Foundation for Research and Technology, Hellas, Institute of Chemical Engineering Sciences, GR-26504, Patras, Greece*

[2] *Foundation for Research and Technology, Hellas, Institute of Chemical Engineering Sciences, GR-26504, Patras, Greece and University of the Peloponnese, Department of Mechanical Engineering, GR-26334, Patras, Greece*

Corresponding Authors: vbur@iceht.forth.gr, nadia@nbali.gr, caggelop@iceht.forth.gr

A numerical model of the plasma formation inside a porous soil material placed in a Dielectric Barrier Discharge (DBD) reactor has been developed. The particulate reactor system comprises of a High-Voltage (HV) electrode in contact with the polluted porous soil, which triggers plasma formation inside the pores of the soil, Fig.1. This reactor type is a step towards an in-situ investigation, where the oxidants will instantly react with pollutants inside the pores. A true-to-mechanism model is implemented for the incorporation of the effect of the porous structure on the plasma equations. For this reason, an analysis to assess the impact of the porous structure on the process has been performed, which is initially applied in a test case model inside an actual DBD reactor. The phenomena

that take place inside the porous structure are studied and their effect on the species transport properties are assessed, for all key species that are formed, such as ions, electrons and neutral species. An Effective Medium Theory (EMT) approach is applied for the species transport properties inside the granular porous media 1. More specifically, the model uses the effective permittivity value derived in pertinent literature 2, as a result of the applied electric gradient inside heterogeneous structures. Moreover, the effective mobility is also used, which determines the charged species motion due to the electric field and follows the so-called Einstein's expression. Additionally, the effective diffusivity value is estimated as a result of the species diffusion inside the porous granular medium under the presence of the rest of the species (initial air composition of 79% N2 and 21% O2). Finally, for the air flow, a Darcy-Brinkmann equation is used for the estimation of the velocity distribution inside the porous soil medium. The air flow model is an effort to simulate turbulence inside porous media, which is currently developed based on the Darcy and non-Darcy permeability coefficients of the Forchheimer equation 3.
A range of applied voltages are tested under various electrical supply conditions, namely under AC, DC, and pulse conditions. In addition, various distances between the anode and cathode electrodes are also considered, and an optimum distance between the HV electrode and the ground is suggested. The results also reveal the influence of species distribution on the production and the remediation rate due to the air flow and the permeability value. This may lead to optimization of the process in view of the flow rate, leading to improved pollutant degradation rate, and of the diverse soil composition (i.e., with varying permeability), which causes different species concentration and, therefore, different electron densities. Finally, the species production is compared with experiments, and the electron density prediction is validated by literature findings [4], as well.
In conclusion, an effective approximation of the DBD reactor plasma and the internal transport phenomena has been developed, which offers valuable insight on the mechanisms of in-situ soil remediation for the optimization of future processes, and saves considerable time and effort from extensive experimentation.

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Porous system characterization of a heterogeneous carbonate rock bed using x-ray microtomography

Authors: Fernanda Hoerlle[1]; William Godoy[1]; Elizabeth May Pontedeiro[1]; Paulo Couto[1]

[1] *LRAP/UFRJ*

Corresponding Authors: bettymay@petroleo.ufrj.br, fernandahoerlle@petroleo.ufrj.br, pcouto@petroleo.ufrj.br, wmgodoy@petroleo.ufrj.br

Coquinas are heterogeneous carbonate reservoir rocks. The characterization of its porous system is essential to determine the flow properties. In this study, we aimed to quantify and qualify the porosity, focusing on the anisotropy and the connectivity, using X-ray microtomography (microCT) images.
Nine coquinas samples were collected across a bed 1 meter high and 9 meters in length. We carried out a petrophysics routine using Helium porosimeter and Nitrogen permeameter. The porosity of

the samples varied from 13.9% to 20.3%, and the permeability from 33.2mD to 765.6mD. For the digital analysis, we imaged the samples with a pixel size of 18μm. The microCT images were segmented according to the Kittler & Illingworth (1986) method, the volume of interest (VOI) was selected, and the digital porosity was calculated. The digital porosity varied from 5.0% to 17.3%.
In the microCT images, the shells, cement, and siliciclastic minerals appear in different scales of grey. The anisotropy of the rocks was observed by the irregularity of the pore space boundary. The shapes of the pores are very heterogeneous in both 2D and 3D. The heterogeneity of samples was also emphasized by the pore size variation from 0.02mm to 2.77 mm in the microCT images, with no predominant pore size pattern.
The anisotropy could also be observed when analyzing the porosity variation through the sample length. There are regions of higher and lower porosity across the samples, and the digital porosity is equivalent to the mean of the porosity through the samples.
From the digital porosity data, it was possible to evaluate the connectivity of the porous system, which was always lower than the digital total porosity. In addition, in some samples, we could not obtain this property, most likely due to the threshold value used to segment the pore space. Another reason could be the image resolution. The pores that are responsible for the connectivity of the porosity are bellow the resolution of the microCT images and could not be observed.
We conclude that the heterogeneity, anisotropy, and connectivity of the porosity in the coquinas samples can be analyzed using microCT images. These properties were observed in each sample but they also occur along the original geological bed. Carbonate rocks are challenging to be characterized and microCT is an important technique that allows evaluating its internal porous structure with detail without damaging the rock.

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Predicting Performance of Offshore Oilfield in High Water Cut Period Based on Big Data and Artificial Intelligence

Authors: Cunliang Chen[None]; Shaopeng Wang[1]; Hongyou Zhang[None]; Yu Wang[1]; Qiongyuan Wu,[None]; Xue Liu[None]

[1] *Tianjin Branch of CNOOC (China) Co., Ltd*

Corresponding Authors: liuxue@zhenhuaoil.com, shidacunliang@126.com

Water drive curve is an important method for predicting performance. Traditional methods are based on exponential formulas, but these methods have poor adaptability in high water cut period. Because traditional methods deviate from straight line in high water cut period. In this paper, a robust method for predicting performance of offshore oilfield in high water cut period based on big data and artificial intelligence is proposed. A new percolation characteristic characterization equation with stronger adaptability is proposed, which focuses on the limit of high water flooding development. On this basis, the equation of the new water drive characteristic curve is deduced theoretically, and the dynamic prediction method is established. What's more, the solution of the method is based on large data and AI algorithm. This method has been applied to nearly 100 high water flooding phase permeability curves, and the coincidence rate is more than 95%. The new water drive characteristic curve can better reflect the percolation characteristics of high water cut reservoirs, and the conventional water drive characteristic curve is a special case of the new water drive characteristic curve when the recovery degree is low. At the same time, the performance of adjustment wells and measures on the curve of development dynamic image is analyzed. Curve

warping indicates that adjustment wells or measures are effective. Field application shows that the prediction error of the new method is less than 5%, which is more in line with the needs of oilfield development. Because of the application of artificial intelligence algorithm, the application is more convenient and saves a lot of time and money. This is a process of self-learning and self-improvement. As the oil field continues over time, each actual data will be recalculated into the database. Then the fitting and correction are carried out, and then the solution is learned again. This method has been applied to several oil fields in Bohai. And the effect is remarkable.

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Mathematical Model of Thermo-Gel Flooding and Its Application in Thermal Recovery of Offshore Heavy Oil

Authors: Jintao Wu[None]; Lei Zhang[None]; Jianting Huang[None]; Hao Li[None]; Guangming Pan[None]

Aiming at the problem that common thermal huff-puff is difficult to achieve economic development at offshore oilfield, a new development method of thermo-gel treatment assisting multiple thermal fluid huff-puff is proposed. This method is based on the temperature to regulate the underground viscosity of thermo-gel, thereby achieving the purpose of reducing the oil-water mobility ratio, replenishing reservoir energy and increasing the inter-well developed reserves. Based on a laboratory experiment, the changing law of thermo-gel viscosity was researched. As the polymer concentration increases, the critical temperature of thermo-gel decreases according to a binomial relationship. Considering the influence of temperature on the viscosity of the solution system, the chemical kinetic reaction, the adsorption of the rock surface and the permeability decrease, a mathematical model was established. A numerical simulation study of non-isothermal chemical flooding was carried out at offshore N oilfield. The main parameters of thermo-gel treatment assisting multiple thermal fluid huff-puff were determined: the reservoir pressure is higher than 8 MPa, the gel injection-production ratio is 1.0 and the thermal huff-puff is over 3 cycles. After the pilot test was implemented, the well production during the first cycle of thermo-gel treatment assisting multiple thermal fluid huff-puff was 60~90m3/d with stable production exceeding 1,000 days. Compared with common thermal huff-puff, the periodic oil production increased by 3.4×104m3 and the period of validity increased by 511 days. The forecast cumulative oil production is increased by 5.3×104m3 and the recovery factor is increased by 4.2%.

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Study on the micro pore structure characteristics of low permeability porous carbonate reservoir

Authors: yapu zhang[None]; zhengming yang[None]; yanzhang huang[None]; xingwang shi[None]; haitao hou[None]

Corresponding Author: 28478341@qq.com

The carbonate reservoirs in the Middle East are mainly of pore type with complex micro pore structure. Taking Middle East H low permeability carbonate reservoir as the research object, this paper systematically studies the reservoir characteristics, fluid occurrence and seepage law of low permeability carbonate reservoir by using constant velocity mercury injection, CT scanning, NMR and low permeability physical simulation, and establishes a five-parameter evaluation method for reservoir classification. (1) H low permeability carbonate reservoir is mainly pore reservoir with a few micro fractures and holes. Pores with diameter less than 2mm account for more than 80% of the volume; the larger the permeability, the wider the radius distribution of the larynx, the greater the contribution of the large throat to the permeability; when the permeability is less than 2 mD, the peak value of the radius of the larynx is 0.5 micron; Compared with the low permeability sandstone reservoir, the low permeability carbonate reservoir has the characteristics of "large pore but small quantity" and "large throat and full type". （2）When permeability of rock sample is less than 5 mD, movable oil mainly comes from mesopore, coarse pore and fine pore, remaining oil mainly exists in mesopore and part of coarse pore; when permeability is greater than 5 mD, movable oil mainly comes from coarse pore, macropore and medium pore, remaining oil mainly exists in coarse pore and part of macropore; there is obvious difference with low permeability sand reservoir, except for small pore, large pore in low permeability carbonate reservoir. Most of the remaining oil still exists in the pore.(3) The five parameter reservoir classification and evaluation results are in good agreement with the current production of six horizons of H oilfield in the Middle East.

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Flow diagnostics for fractured reservoirs: An innovative way to account for geological and geomechanical uncertainty in modern reservoir modelling and simulation workflows

Authors: Sebastian Geiger[1]; Victoria Spooner[1]; Lesly Gutierrez Sosa[1]

[1] *Heriot-Watt University*

Corresponding Authors: lmg1@hw.ac.uk, ves1@hw.ac.uk, s.geiger@hw.ac.uk

Fractured reservoirs are abundant in the subsurface and crucial to the provision of energy (e.g. oil, gas, geothermal) and groundwater, as well as for the storage of CO_2. Yet, these reservoirs are very difficult to characterise, develop, and manage due to their complex and uncertain geology. Fractures can also open or close as the stress state in the reservoir changes during production, adding further complexities to the reservoir management. Modern reservoir simulation and uncertainty quantification workflows allow us to support the design of field development and management plans that account for geological uncertainties. However, simulating these reservoirs is not trivial and the time spent running full-physics reservoir simulations is valuable; it should be used for studying models that explore a realistic range of (geological) uncertainties and hence provide the most insight.

We have developed new flow diagnostics tools for naturally fractured reservoirs which sacrifice some physical detail in exchange for speed but still allow us to compute some of the essential dynamic behaviours in the reservoir, e.g. how effectively wells communicate with each other or which wells are at risk of early breakthrough. A particular innovative addition to our flow diagnostics is that we can also account for geomechanical effects in the reservoir; we can therefore quickly evaluate if and where fractures are likely to open or close, and how reservoir dynamics evolve as a consequence, due to production-induced stress changes.

Our new technology enables us to screen large numbers of geological models based on their approximate dynamic and geomechanical behaviours in a matter of minutes prior to commencing more

time-consuming full-physics reservoir simulations. Using intuitive metrics we quantify the reservoir dynamics to cluster models and reduce the number of full-physics simulations required for robust reservoir forecasting without affecting the original range of geological and geomechanical uncertainties. Flow diagnostics hence offer a natural pre-processing step that complements modern coupled hydro-mechanical reservoir simulation, uncertainty quantification, and optimisation workflows, allowing us to spend valuable simulation time on the cases that yield a greatly improved understanding of reservoir performance and related uncertainties.

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Liquid-gas penetration through the complex three-dimensional porous media

Authors: Yu Shi[None]; Xiao-na Yang[None]

Corresponding Author: shiyu@xust.edu.cn

The dynamic behaviors of liquid-gas penetration in porous media are important for many situations, such as water imbibition, drainage, and chemical agents absorption in rock. In this work, the multiphase-lattice Boltzmann model which demonstates the capability in handling multiphase flow with large density ratio is employed to investigate the two-phase flow at the pore-scale level in complex porous media. The results show that the droplet can penetrate through the porous meida swiftly with the increase of porosity. It is easier for the liqiud to transport in the hydrophobic porous media because of the lubricating effect of the thin gas film. Increasing density ratio leads to a higher penetration rate due to larger kinetic energy conversion from the gravitational potential energy. Furthermore, the decrease of interfacial tension causes more scattering of the liquid, whereas the increase of viscosity ratio leads to a postponed liquid penetration. Moreover, the liquid penetration is promoted in pores which in parallel to the gravitational force. On the contrary, the pores perpendicular to the driven froce exert much resistance to the fluid flow.

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Reservoir Parameter Changes of Weakly-Volatile Oil Reservoir Developed by Natural Energy and The Potential Analysis of Water Injection: A Case Study of Offshore X Oilfield

Authors: Jianting Huang[None]; Jintao Wu[None]; Guangming Pan[None]; Hao Li[None]; Zhenpeng Li[None]

Corresponding Author: huangjt@cnooc.com.cn

For volatile reservoirs, pressure maintaining production is adopted as common. Limited by the early offshore special development condition, X oilfield, an offshore weakly-volatile oil reservoir, has been developed by natural energy for up to 7 years. In order to improve the effect of oilfield development, its reservoir parameter changes and water injection potential need further study. Based on the laboratory core and physical model experiments, this paper studied the changes of reservoir formation parameter and oil phase state of X oilfield after the natural energy development. The results show

that the porosity has dropped to 98.5% of the initial porosity and the permeability has dropped to 86.5% of the initial permeability as the formation pressure has dropped by 15MPa. The permeability is more sensitive to the formation pressure compared with the porosity. At the same time, the phase state of crude oil changed obviously. The gas oil ratio decreased from 221m3/m3 to 80m3/m3, the viscosity of formation oil increased from 0.35mPa·s to 0.61mPa·s, the mobility of formation oil decreased from 257 mD/mPa·s to 128 mD/mPa·s and the flow capacity of formation oil decreased by 50%.

In order to characterize the potential of water injection under different conditions, the artificial model of aluminophosphate quartz sand is used. Five injection conditions are compared in the scheme design, which are: (1) direct water injection under the original formation pressure of 30.5MPa; (2) direct water injection under the bubble point pressure of 28.9MPa; (3) natural energy development to 24MPa and then water injection; (4) natural energy development to 18MPa and then water injection; (5) natural energy development to 12MPa and then water injection. In order to ensure the accuracy and reliability of the experimental comparison, the average initial oil saturation of the five experimental models is 56.43% and the deviation is between 2.63% and 0.39%. The experiment shows that the total displacement efficiency of water drive is the highest when the bubble point pressure is reached. And then the lower the pressure is, the lower the total displacement efficiency is. When the time of water injection is later, the displacement efficiency of dissolved gas drive is higher, the displacement efficiency of water drive is lower and the total displacement efficiency is lower.

Based on the potential analysis results, the water injection was carried out at X oilfield. The formation pressure gradually increased with the increasing rate of 8.4%. The decreasing rate of the oil production was reduced from 20.8% of the natural energy development stage to 4.1% of the water injection stage. The field practice shows that the water injection is an effective method to improve the recovery of weakly-volatile reservoir.

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Molecular dynamics simulation of methane and water molecules in the ultramicro channels of graphene and modified graphene

Author: Zeyuan Wang[1]

Co-authors: Yaxue Zhang [1]; Shujun Chen [2]; Yue Fu [3]

[1] *College of Pipeline and Civil Engineering, China University of Petroleum (East China)*

[2] *College of Pipeline and Civil Engineering, China University of Petroleum (East China); Shandong Key Laboratory of Oil & Gas Storage and Transport Safety; Qingdao engineering research center of efficient and clean utilization of fossil energy*

[3] *College of New Energy, China University of Petroleum (East China)*

Corresponding Authors: shujunchenfu@126.com, fuyuefy@126.com, 1649038803@qq.com, upcwzy@163.com

At present, how to realize the high density storage of natural gas is the main technical factor restricting the large-scale application of natural gas.1 LNG and CNG technology are more industrialized, but they have the disadvantage of high energy consumption.2 Natural gas storage by hydrates is a new solution in natural gas storage and transportation industry.3 It is found that the use of nanoparticles is very effective in accelerating the formation of hydrate and increasing the storage capacity of methane.[4,5] Graphene is a kind of porous media material with wide application prospect. Some studies have shown that graphene nanofluids can reduce the induction time of methane hydrate and increase methane storage.[6,7] When the pore width of graphene nanoparticles is less than 1.2nm, it is difficult for methane hydrate(unit cell is about 1.2nm) to form in the ultramicropore. In this case, the adsorption and diffusion of methane and water will occur in the ultramicropore, but the movement behavior is not clear still. At the same time, for the ultramicropores with limited pore width of 0.6 nm-1.5 nm, the structure and dynamic behavior of water will change obviously.[8]

In this study, the properties of adsorption and diffusion kinetic of water and methane in the ultramicro channels of graphene modified by different groups are studied. We constructe nine systems composed of water, methane and water/methane mixed system with graphene, hydroxyl modified and amino modified graphene. The pore widths of the three graphenes are 0.8nm. Molecular dynamics simulations are conducted to study the adsorption properties and kinetic properties included radial distribution function, mean square displacement and diffusion coefficient of water and methane in the ultramicro channels of graphene, hydroxyl modified and amino modified graphene. The results show that in terms of adsorption properties, when the methane/water mixture simultaneous diffuse into ultramicro channels of graphene and modified graphene, amino modified graphene is more beneficial to increase methane storage and reduce the adsorption capacity of water. Compared with unmodified graphene, the presence of water limits the movement of methane and make methane stably stays in the ultramicro channels of modified graphene. In terms of diffusion properties, compared with the single component, the diffusion coefficient of water in the mixed system increases obviously and water diffuse more violently in the three kinds of graphenes, while the modified graphenes inhibit the movement of methane in the mixed system and the diffusion coefficient is reduced. The kinetic properties of restricted guest molecules in the ultramicro channels are related to the degree of order. Based on the comprehensive analysis of the adsorption and diffusion properties, it is concluded that among the three kinds of graphenes, amino modified graphene is more suitable for the study of natural gas storage by hydrate method. The results of this study are helpful to understand the micromolecular mechanism of methane and water molecules diffusion in the ultramicropore of graphene and provide theoretical guidance for the design of excellent materials for natural gas storage by hydrate method.

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A Prediction Model for Relative Permeability Curve Based on Improved BP Neural Network Using Bayesian Regularization

Author: yanhui Zhang[None]

Co-authors: Yingxian Liu ; Hui Cai ; Jiang Lifu ; Hongyou Zhang

Corresponding Author: zhangyh27@cnooc.com.cn

For the reservoirs with strong heterogeneity, the relative permeability curve is different for different reservoir horizon or position. Correcting and predicting the endpoint value of relative permeability curve based on reservoir permeability and porosity is one of the keys to improve the accuracy of reservoir numerical simulation. However, there is a complex nonlinear relationship between reservoir permeability and the endpoint values of the relative permeability curve. Therefore, a BP neural network method is proposed to predict the endpoint value of relative permeability curve by permeability and porosity. The BP neural network model is improved by Levenberg-Marquard algorithm. Porosity and permeability of the 149 relative permeability curves are the input variables, endpoint values of the 149 relative permeability curves (irreducible water saturation, residual oil saturation and residual oil saturation of water phase permeability) are the output variables. The difference between the conventional BP neural network and the improved Levenberg-Marquard BP neural network was compared. The results show that the improved BP model has strong nonlinear fitting ability which can truly reflect the nonlinear relationship between the relative permeability curve and permeability. The accuracy of the model is tested with 14 other relative permeability curve data. The results show that the absolute error of the model is within 0.03 and the relative error is less than 5%. This method is used to predict the relative permeability curves of BZ reservoir. The permeability of BZ reservoir are between 200 mD and 3500mD. According to the distribution of permeability and porosity, six relative permeability curves were predicted and six relative permeability curves is consistent with actual the dynamic characteristics of different reservoir horizon or well groups.

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One-domain approach for inertial momentum transfer between a free fluid and a porous medium: two-dimensional flow

Authors: J. Alberto Ochoa-Tapia[1]; Roel Hernandez-Rodriguez[1]; O. A. Luévano-Rivas[1]; Fátima Callejas-Quiroz[1]

[1] *Universidad Autónoma Metropolitana*

Corresponding Authors: fatimadv08@hotmail.com, iqrhr@hotmail.com, iq.luevano@gmail.com

The momentum transfer between a free fluid and a porous medium is found in many applications, including chemical engineering processes, natural systems, among many others. Due to the separation of characteristic lengths and the complex geometry of a porous medium, these types of systems are usually studied by means of effective medium equations. In that context, one of the main difficulties is to describe the momentum transfer in the free fluid/porous medium inter-region. An alternative approach for this is known in the literature as the one-domain approach (ODA), which considers the system as a pseudo-continuum and the momentum transport is described by a generalized transport equation (GTE) valid everywhere in the system (i.e., in the homogeneous free fluid, in the homogeneous porous medium, and the inter-region) (Goyeau et al., 2003). To this end, the GTE considers position-dependent effective medium coefficients. However, up to now the physical meaning of such coefficients is not well understood, so heuristic interpolations are frequently used, which do not guarantee that such equations can provide an accurate description of the physical processes. In addition, most studies of momentum transfer between a free fluid and a porous medium are limited to the study of unidirectional and Stokes flow problems. In this work, we used a GTE obtained by applying the volume averaging method on the pore-scale equations for the incompressible and inertial flow of a single-phase between a free fluid and a porous medium. These equations are in terms of an apparent permeability tensor and a total inertial tensor, which can be predicted by solving the associated local closure problem. As a study case, we considered the two-dimensional flow in a rectangular cavity partially filled with a porous medium (Luminari et al., 2019). Through the solution

of the local closure problem, in a representative element of the free fluid/porous medium system, we obtained the closed form of the GTE. Also, we analyzed the two-dimensional dependence of the effective medium coefficients on the Reynolds number and the microstructure of the porous medium in the inter-region. Our results show that the two-dimensional average velocity profiles, obtained from the averaging the local velocity profiles, can be reproduced by those obtained from the solution of the ODA used in this work, without the need of heuristic interpolations to predict the effective coefficients. Finally, it is worth stressing that, the importance of the predictions of the effective coefficients transcends until the determination of those associated coefficients with the jump boundary conditions, which is another modeling alternative for the momentum transfer between a free fluid and a porous medium.

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Statistical Model for Mineral Nucleation and Growth

Authors: Helge Hellevang[1]; Mohammad Nooraiepour[2]; Mohammad Masoudi[3]; hossein fazeli[4]

[1] *Department of Geosciences, University of Oslo*

[2] *University of Oslo (UiO)*

[3] *University of Oslo, Department of Geosciences*

[4] *University of Oslo*

Corresponding Authors: hossein.fazeli@nottingham.ac.uk, mohammad.masoudi@geo.uio.no, helge.hellevang@geo.uio.no, nooraiepour@gmail.com

Nucleation is the first step in the precipitation process, and it controls where in the pore space crystal growth occur. The spatial distribution of stable secondary nuclei and crystals has a major effect on the porosity-permeability relation, and it is therefore vital to also include nucleation in reactive transport models. There are few reactive transport models taking into account the nucleation process and in these models nucleation occurs after concentration reaches certain threshold values. Mineral nucleation is however a statistical process, where the probability of crystal nucleation is given by the physical conditions (surface characteristics, supersaturation, temperature, etc) at the substrate-solution interface.
We have developed a new probabilistic nucleation model and incorporated it into a pore-scale reactive transport solver to simulate mineral nucleation and growth and the effect on the porosity-permeability relation of porous media. The nucleation rate in the new model can be either approximated from classical nucleation theory (CNT) or provided by experimental data. In this work, we used experimental data. Laboratory experiments using polished rock-chips provides us with the spatial distribution of crystals and the total number forming per surface area at varying temperatures, supersaturations and time. This can in turn be translated to the induction time of stable nuclei for the given substrate, which can be tabulated and used in the numerical simulations. Laboratory experiments demonstrate that surface roughness of the substrate is a critical factor affecting the interfacial free energy and thereby the induction time.

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Reservoir characterization and pore size distribution: An evaluation for the Eocene Beach-Bar Sequence, Dongying Depression, China

Author: Muhammad Aleem Zahid[1]

Co-authors: Chunmei Dong [2]; Alexandra N. Golab ; Chengyan Lin ; Zhang Xianguo ; Xinmin Ge ; Songtao Wu ; Muhammad Jawad Munawar ; Cunfei Ma ; Knuefing Lydia

[1] *Lasbela University, Pakistan*

[2] *China University of Petroleum, Qingdao, China*

Corresponding Authors: lcydcm@upc.edu.cn, z_aleem@live.com

Abstract Pore size distribution and associated heterogeneities of thinly bedded beach-bar sandstone reservoir from upper fourth member of EoceneShahejieFormation(Es4s)arecharacterizedwiththehelpofmercuryinjectioncapillar resonance(NMR)transversalrelaxationtime(T2)data.Permeabilityandporosityaretworepresentedimportantcharacteristicsofrock that control the movement and storage of fluids. The aim of this paper is to establish relationships between pore throat sizes and reservoir quality.The resultsderived from thin-sectionpetrography,scanningelectronmicroscopy (SEM),MICP,NMRT2 relaxation time, and 3D micro-CT (μ-CT) are compared to characterize pore space dimensions and types comprehensively. Average pore throat size from MICP ranges between 0.47 μm and 2.83 μm while maximum pore throat size ranges between 2.48 μm and 7.36 μm. The combinationofporesizedistributionobtainedfromMICPandNMRseemsappropriatetocovertherangeofporesizefrombeach-bar sand and overcome the individual method limits. Afterwards, digital 3D μ-CT tomographic images are used to characterize and visualize pore space and pore network model to compare with the experimental data. MICP and NMR experiment showed generally bimodal (meso and micro) pore size distribution. Usually mesopore corresponding to intergranular pores is dominant, while heavily cemented sandstones show large amounts of intercrystalline micropores. Complex and heterogeneous beach-bar sandstone reservoir requires comprehensive study program to evaluate the reservoir.
Keywords NMRT2 .MICP.Poresizedistribution .Porosity .3Dμ-CT .Porenetworkmodeling

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Analysis of Viscous Fingering for Steam Flooding Heavy Oil Reservoirs

Authors: Xue Liu[1]; Jing Huang[2]; Xiangyun Qu[1]

Co-authors: Ming Li [1]; Ming Jiang [1]; Xianming Kou [1]; Enshun Ouyang [1]

[1] *China zhenhua Oil Co., Ltd*

[2] *CNOOC Research Institute*

Corresponding Author: liuxue@zhenhuaoil.com

Steam drive has been a frequently-used method to enhance heavy oil reservoirs recovery. In the process of steam displacement, the fluid flow area can be divided into three zone, steam zone, steam-oil zone and oil zone respectively. However, piston displacement is difficult to get it due to the difference in mobility between steam and oil. This difference significantly inhibits the heavy oil recovery. This paper contrast and analyzed the effect of the different steam parameter, and based on this, reasonable parameters to enhance oil recovery can be determined.
Based on the thermal equilibrium principle and the relationship of the average gas steam saturation to temperature in the steam-oil zone, a mathematic model is established to analyze formation and evolution of viscous fingering in heavy oil recovery process by steam flooding. During the solving process, viscosity profile of crude oil is modified by using the iteration method. Velocities of steam and oil at the displacement front of two-phase are separately obtained. Then the development of viscous fingering is described by their velocity contrast. Additionally, this study analyzed effects of the viscosity reduction features of steam, steam dryness, steam temperature and displacement velocity on performance of viscous fingering.
The results show that viscous fingering would be prevented by oil viscosity reduction in steam flooding. Viscous fingering would also become weak with increase of steam dryness. However, with increase of steam temperature or displacement velocity, viscous fingering would become worse. In order to control the viscous fingering and enhance heavy oil recovery in steam flooding, steam dryness should not be less than 0.6. Steam temperature should not be lower than 200˚C. In addition, displacement velocity should be within a reasonable range.

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Real-time Synchrotron-Based X-ray computed microtomography during in situ emulsification

Author: Yara Alzahid[1]

Co-authors: James McClure [2]; Cheng Chen [3]; Peyman Mostaghimi [4]; Ryan Armstrong [4]; Chenhao Sun [4]

[1] *EXPEC Advanced Research Center*

[2] *Advanced Research Computing, Virginia Tech, Blacksburg, Virginia, USA*

[3] *Department of Mining and Minerals Engineering, Virginia Tech, Blacksburg, Virginia, USA.*

[4] *UNSW*

Corresponding Author: yara.zahid@aramco.com

Molecular-level forces experienced by a surfactant during emulsification can have a significant impact on emulsion structure and effective properties. Understanding the interplay of molecular-level forces and effective phase properties during in situ emulsification is a fundamental question relevant to various subsurface engineering applications. Herein, we use dynamic synchrotron-based X-ray microtomography to capture flow dynamics during an oil emulsification process, whereby brine salinity influences the predominate molecular-level forces. We measure oil recovery, phase viscosities, phase morphologies, contact angles and water relative permeability to elucidate the underlying oil recovery mechanisms. Optimum salinity formed a stable emulsion phase with ultra-low interfacial tension, viscosity high enough to reduce the mobility of the injected solution and a reduced adhesive force that resulted in less contact between oil and solid grains. These mechanisms are attributed to favorable flow dynamics that lead to improved oil recovery that can be tuned by brine salinity.

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Pore scale simulation of solute transport in immiscible two phase flow system

Author: Zhang Chunwei[1]

Co-author: Tetsuya Suekane [1]

[1] *Tokyo Institute of Technology*

Corresponding Authors: tsuekane@es.titech.ac.jp, zhang.c.aq@m.titech.ac.jp

The transport of nonreactive dissolved chemical species through two phase systems can be found in multiple engineering applications, such like contaminants remediation and enhanced hydrogeological resources recoveries. The solute dispersion in a single fluid particle system can be deemed as an interplay between molecular diffusion and advection flow along the tortuous flow path. However, it is much more complex for the immiscible two phase system, where the distribution of the aqueous phase and the resulting hydrodynamic flow field might add a profound influence on the dispersivity of the passive tracers. In this work, we numerically study the two phase flow in a randomly packed glass beads through the Shan-Chen psudopotential MRT lattice Boltzmann method (LBM). The simulated sample is reconstructed from high resolution Micro–CT images that is representative of the real porous structure. Then, the solute transport process in the aqueous phase is simulated using a mass transport LBM scheme. While fixing the Péclet number to a constant of 1000, a temporal tracer concentration profile is obtained over a range of the aqueous phase saturation Sw from 0.17 to 0.93. We successfully discover the anomalous solute transport behaviours that show a dependence on Sw. The fingering like preferential flow path and stagnant zones are recognized. The scalar dissipation rate and the dilution index are thoroughly investigated to describe the mixing state. The result can be used to elucidate the solute transport behaviours in the two phase system.
Keywords: Two phase flow; dispersion; LBM; Aqueous phase saturation; Scalar dissipation rate.

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Adsorption and Diffusion of Water in Zeolitic Imidazolate Framework-8: Effect of Structural Flexibility

Author: Zeyuan Wang[None]

Co-authors: Yaxue Zhang ; Shujun Chen ; Xuejian Li ; Yue Fu ; Jianlin Pei

Corresponding Authors: shujunchenfu@126.com, fuyuefy@126.com, 1435196975@qq.com, 374114475@qq.com, 1649038803@qq.com, upcwzy@163.com

Metal-organic frameworks (MOFs) are promising candidates as natural gas adsorbents due to their porous feature and high structural tenability.1 Among them, ZIF-8 has received extensive attention in gas storage and separation due to its unique flexibility.[2-4] In terms of natural gas storage, several simulation studies have been conducted to examine adsorption and diffusion of CH4 and CO2 in ZIF-8, and considered the flexibility of its framework.[5-8] However, because natural gas often contains a certain amount of water,[9] it is necessary to consider the adsorption and diffusion properties of water in ZIF-8, but there are few studies in this area, and the effect of structural flexibility on water transport properties is not clear.
In this study, we study the transport properties of water with different loadings in rigid and flexible ZIF-8 frameworks, including adsorption and diffusion properties, by equilibrium molecular dynamics (MD) simulation. We find that water would form clusters and then compared the effects of cluster formation in rigid and flexible framework on methane adsorption by grand canonical Monte Carlo

(GCMC) simulation. ZIF-8 uses flexible force field to consider flexibility.5 For a rigid framework, we fix the atoms in their initial position and keep them at rest. Our findings are mainly in the following aspects: (1) In both rigid and flexible framework, water molecules form clusters through hydrogen bonds in the pore cavity, and the number of clusters is related to the loading amount of water. They are easier to form in the adjacent pore cavity. The formation rate of clusters is slow in the rigid framework, while in the flexible framework, water molecules gather and form clusters faster because of the swing of the imidazole chain, which is consistent with the change trend of potential energy. (2) In the rigid framework, the self-diffusion coefficient of water increases monotonously with the increase of water loadings. This loading dependence satisfies the type Ⅲ self-diffusion process.[10] The reason is that water molecules capture isolated water through strong hydrogen bonds and pull its motion, resulting in the formation of clusters and a low share in the channel. However, there is a huge difference in flexible framework. With the increase of the loading, the diffusion coefficient first decreases and then increases. Especially when there are less than 5 water molecules per unit cell, The diffusion coefficient is about 100 orders of magnitude of rigidity. This finding is verified by comparing the radial distribution functions of water (Ow) and the main adsorption sites (C2, Zn) of rigid and flexible frameworks. The movement of ZIF-8 atoms keeps the water molecules away from the adsorption site. (3) in addition, through the GCMC simulation, we find that the formation of water clusters slightly inhibit the methane adsorption in the pressure range of 0-6MPa, and the rigid and flexible framework have no effect on the methane adsorption. The results of this study are helpful to understand the effect of structural flexibility on water transport properties and provide theoretical guidance for the design of excellent materials for adsorption gas storage.

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Experimental Study on the Effect of Injection-production Well Spacing on Distribution of Remaining Oil in Offshore Polymer Flooding Thick Reservoirs

Authors: Guohao Zhang[1]; Zongbin Liu[1]; Yanlai Li[1]; Zhaobo Sun[1]

[1] *Tianjin Branch of CNOOC Ltd.*

Corresponding Author: zhanggh21@cnooc.com.cn

Injection-production well spacing determines the cost and effect of oilfield development, and has remarkable influence on the distribution law of remaining oil. The development cost is high for offshore oilfields, thus reasonable well pattern and well spacing are needed in both water flooding and chemical flooding reservoir. In order to clarify the influence of injection-production well spacing on the distribution of remaining oil in offshore thick reservoirs, two-dimensional visual physical models with different injection-production well spacing were made, and displacement experiments such as water flooding and polymer flooding were carried out, and distribution law of remaining oil was analyzed.

Two kinds of injection-production well spacing was preliminarily designed in the experiment which is 28cm and 50cm, respectively. There rhythm modes were considered, which were homogeneous rhythm (average permeability is 1500mD), positive rhythm (600/1500 / 1900mD) and reverse rhythm (2400/1500/800mD), a total of 12 sets of displacement experiments were conducted.

The experimental results showed that: 1. Sweep efficiency and recovery rate of water flooding and polymer flooding in homogeneous rhythm, positive rhythm and reverse rhythm reservoirs increased with the decreasing of injection-production well spacing, and the recovery rate increased from 4.0% to 20.6%. 2. For homogeneous rhythm reservoir, injected water rapidly broke through along bottom due to gravity differentiation, while polymer flooding could mitigate the effect of gravity differentiation and improve sweep efficiency to a certain extent, but remaining oil enriched in the top of the reservoir around production wells in both water flooding and polymer flooding modes. As the injection-production well spacing decreased, polymer flooding could further improve the sweep efficiency of the top of the reservoir and further enhance the recovery rate by 20.6%. 3. For positive rhythm reservoir, influenced by gravity differentiation and reservoir heterogeneity, water breakthrough phenomenon was more serious than that in homogeneous rhythm reservoir, and polymer flooding improved the production of middle-permeability layers, thus remaining oil in middle-permeable layers which mainly distributed in the top of low-permeability layers around the production well was largely recovered. With the decreasing of injection-production well spacing, remaining oil in top of low-permeability layers was further swept by polymer flooding and recovery rate was further enhanced by 11.7%. 4. For reverse rhythm reservoir, the swept degree of water flooding was more uniform. Remaining oil mainly accumulated in local area which was not swept and top layers around production well, and polymer flooding further improved swept efficiency. With the decreasing of injection-production well spacing, the overall swept degree of polymer flooding was more uniform, and the recovery rate was further increased by 15.0%.

Surprisingly, the effect of gravity was remarkable whether applying water flooding or polymer flooding. Basically, the bottom layer produced more and in some flooding processes, the upper layer only produced for a short time and stopped producing due to interference. Therefore, we must attach importance to dynamic interference and other issues in the development process. The results of this research can guide the polymer flooding development and remaining oil tapping after polymer flooding in offshore oilfields.

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Pore-scale experimental investigation of the effect of wettability heterogeneity on interfacial area in three-dimensional porous media

Authors: Yingxue Hu[1]; Tetsuya Suekane[2]

[1] *Department of Mechanical of Engineering, Tokyo Institute of Technology*

[2] *Department of Mechanical Engineering, Tokyo Institute of Technology*

Corresponding Authors: tsuekane@es.titech.ac.jp, hu.aa@m.titech.ac.jp

Wettability is an important factor that controls the flow and spatial distribution of fluids in porous media and macroscopic multiphase properties. The trapped cluster distribution from singlet to multiple further affects the interfacial area. As mass transfer is localized to the fluid-fluid interfacial area, namely meniscal interfacial area, the ratio of meniscal and total interfacial area affects the rates of mass transfer. The objective of this study was to investigate the effect of wettability heterogeneity on interfacial area of trapped phase in three-dimensional porous medium using X-ray microCT. Water-wet and intermediate-wet glass beads were mixed with specifically fraction (water-wet volume fraction fw = 0, 20%, 40%, 60%, 80% and 100%) to produce the synthetic porous media. Brine was injected with four different flow rates (Capillary number Ca ranging from 1×10-6 to 3×10-4) to produce the second imbibition in the above porous media. The trapped phase was visualized and analyzed based on the high resolution images obtained from micro tomography. Findings indicate that residual saturation, cluster size distribution and interfacial area are influenced by the wettability heterogeneity in three-dimensional porous media. Heterogeneous wettability distribution of particle surface leads to more residual cluster, suppressing the connectivity of trapped phase. Small size singlet owns a higher ratio of meniscal and total interfacial area than larger size ganglion. Thus, heterogeneous wettability porous media contributes a higher meniscal interfacial area, resulting in a fast dissolution rate. Results of this study may can enrich the understanding the non-aqueous phase liquids and gas removal from groundwater.

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Research and field case on injection parameter optimization of surfactant-polymer flooding

Authors: Xinran Wang[1]; Zongbin Liu[1]; Lina Yang[2]; Wei Zhang[1]; Zhanfeng Li[1]; Zhaozhao Qu[1]; Guanglong Li[1]

[1] *Tianjin Branch of CNOOC (China) Ltd.*

[2] *CNOOC EnerTech - Drilling & Production Co. Ltd.*

Corresponding Author: wangxr7@cnooc.com.cn

Surfactant-polymer flooding field tests are only conducted in Jinzhou Z Oilfield in Bohai Bay of China at present, the concentrations of surfactant-polymer agent of all injection wells are the same in the early original scheme. With the high speed of offshore oilfield development, the production characteristic of different well groups also different greatly, the same concentration isn't in line with the practical oilfield. It is urgent to optimize the injection parameters of the original scheme.
In order to enhance the effect of surfactant-polymer system, better matching of different well group, based on the theory of mobility control, a formula for calculating oil-water relative permeability under low interfacial tension is derived, which by using the method of relative permeability curve treatment under low interfacial tension. Combining with the description of polymer parameters

changes, the mathematical model of mobility control of surfactant-polymer flooding is established, and the chart of mobility optimum design is also drawn. Field case in Jinzhou Z oilfield show the new method can provide theoretical basis for optimizing injection parameter conveniently and quickly.
According to the results of this research, the following conclusions can be obtained: (1) under the same interfacial tension, the higher the water saturation is, the higher the relative permeability of oil-water mixing zone in flooding front is, and the higher the minimum polymer solution concentration required for mobility control is. It is necessary to accurately estimate the water saturation in the reservoir, the injection parameter optimization design should be based on specific reservoir; (2) under the same polymer solution concentration, the lower the water saturation, the higher the interfacial tension corresponding to the mobility control, and the lower the minimum surfactant concentration required. It is necessary to consider the extent of reducing oil-water interfacial tension by surfactant-polymer system, ensure the result of injection parameter optimization is more in line with field production; (3) taking Jinzhou Z oilfield as an example, within the water cut range from 79.4% to 92.8%, the minimum concentration of polymer and surfactant that control the mobility of surfactant-polymer flooding was obtained, and the corresponding chart were made. According to the water saturation of reservoir and the minimum interfacial tension of surfactant-polymer flooding system, the injection parameters can be optimized efficiently.
The innovation of this work is the new idea that the injection concentration should be different under different water cut stage. Based on the theory of mobility control, an optimization model for surfactant-polymer flooding was established. This method has significantly improved the development performance in Jinzhou Z oilfield, compared with the original scheme, the oil recovery increment forecasted is 1.6%, and the chemical agents of surfactant and polymer forecasted saved by 536 tons.

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The effects of oxidation on the capacity of shale gas desorption and diffusion in nanoscale pores

Authors: Yang Zhou[1]; Lijun You[1]; Yili Kang[1]; Qiuyang Cheng[1]; Yang Chen[1]

[1] *Southwest Petroleum University*

Corresponding Authors: youlj0379@126.com, 2536663662@qq.com, 724322467@qq.com, cwct_fdc@163.com, zhouy2020@126.com

The multi-scale fractures formed by hydraulic fracturing provide transport channels for shale gas production. However, the gas in shale nanopores is mainly produced by diffusion, and the gas supply capacity is far lower than the gas flow capacity in fractures, resulting in a rapid production decline. During the development of shale gas reservoirs, the fluids used for fracturing is exposed to air for a long time, which usually contained a large amount of dissolved oxygen(8.0~9.0 mg/L). As a result, a large amount of oxygen enters the shale reservoir with the fracturing fluids. As organic-rich shale is usually formed in anoxic sedimentary environment, it is rich in organic matter and reductive minerals (such as pyrite chlorite). The reductive minerals are easy to react with dissolved oxygen by oxidation, releasing a large number of SO42- and Fe3+, which is easy to produce iron-bearing precipitation and insoluble sulfate precipitation, thus inducing the blocking of shale nanopores and damaging the diffusion capacity of shale gas. By observing the field emission scanning electron microscope (FESEM) images of shale after contact with dissolved oxygen, the damage capacity of oxidation to nanopore was confirmed, and the damage degree of oxidation to shale gas diffusion capacity was 54.5% through the test of gas diffusion coefficient.
This article explored the new method of oxidative fracturing to solve the damage of dissolved oxygen. By adding oxidizing fluid to the hydraulic fracturing fluids, the method can not only break shale with the hydraulic fracturing technology, but also break shale with the oxidation reaction. A large number of fracturing fluids are retained to allow sufficient reaction time and space for oxidizing fluids, which is the engineering basis for the implementation of oxidative fracturing.
The proportion of adsorbed gas in shale is 20%~85%. The adsorbed gas mainly occurs in the organic nanopores. The transport mechanism of the adsorbed gas is mainly desorption-diffusion and slippage flow. Compared with the free methane in larger scale space, the adsorption gas has lower production rate and production degree.
During oxidative fracturing, the organic matter is consumed in large quantities, which can greatly reduce the ability of shale gas adsorption. Meanwhile, oxidation reaction can also generate lots of heat. Under the influence of these two effects, the desorption capacity of adsorption gas in shale nanopores is improved. Large amounts of organic matter and pyrite are dissolved by oxidation reaction, which will produce large number of dissolved pores and fractures, improve the gas supply capacity of the pore throat of the shale block to the fracture system, induce the expansion and extension of shale micro-fractures, shorten the gas transport path in the shale block, so as to relieve the damage of dissolved oxygen and improve the recovery rate of shale gas reservoirs.

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Non-classical hygrothermoelastic response of a hollow cylinder

Author: Zhangna Xue[None]

Corresponding Author: xueangel168@126.com

In dealing with the hygrothermal flow in the high-rate heating process, the propagation characteristics of hygrothermal wave become dominant. By extending the classical Fourier heat conduction law and Fick diffusion law, a hyperbolic hygrothermal coupled model is newly proposed to investigate the hygrothermoelastic response of a hollow cylinder. The cylindrical system is subjected to a hygrothermal shock at the inner surface, and its outer surface is insulated and damp-proof. The integral transform technique and decoupling technique are used to solve the hygrothermal boundary problem. Finally, the effects of hygrothermal coupling, thermal and moisture relaxation time on the transient temperature, moisture, and stress are calculated. It is found that the hyperbolic model gives more conservative results than the parabolic model for the safety design of structures under hygrothermal loads.

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Fractal description of wormhole porous media after acidification

Authors: Hewen Zhang[1]; Honglan Zou[1]; Mingyue Cui[1]; Chong Liang[1]

Co-authors: Anle He [1]; Xuemei Yan [1]; Haibo Li [1]; Yuping Sun [1]; Hongge Jia [2]; Shuzhen Zhang [3]

[1] *Research Institute of Petroleum Exploration & Development*

[2] *CNPC Aktobe Oil & Gas Company*

[3] *CNPC Tarim Oil Company*

Corresponding Authors: hal69@petrochina.com.cn, etczhanghw@163.com, jiahongge@cnpc-amg.kz, zhanghewen69@petrochina.com.cn, cmy69@petrochina.com.cn, lihaibo05@petrochina.com.cn, sunyuping01@petrochina.com.cn, zouhl69@petrochina.com.cn, yanxuemei69@petrochina.com.cn, liangc@petrochina.com.cn

Matrix acidization is one of the most widely practiced and most cost-effective technique to stimulate the production in carbonate reservoirs. As a typical feature in the process, wormholes are formed. Due to the sensitivity of acid-rock reaction to multiple factors, and diverse morphology and random growth of wormholes, there is no quantitative description method available for wormholes, which mainly includes the determination of single wormhole morphology and the distribution of multiple wormholes. These are the preconditions for optimizing the operational design and economically developing such reservoirs.

The short-core flow experimental facility was used to observe the wormholes. CT scan technique was used to describe and observe the morphology of wormholes more intuitively. Then, a square was used to cover the wormhole and divide the wormhole into a series of boxes to obtain the fractal dimension. Besides, a super large core radial flow experiment results were also analyzed in the same way. According to the results of experiments, the fractal calculation model of the wormhole equivalent length and dual-fractal model of wormhole distribution was established.

The pore distribution and wormhole propagation form were obtained. With fractal geometry, different fractal dimension of linear and radial flow wormhole morphologies were proven and calculated. According to the results of experiments, in combination with material balance equations, the wormhole equivalent length model of single wormhole was established, which is the first time to get wormhole length with theoretical calculation. Furthermore, by analyzing the distribution of wormholes,there is a good linear relationship between the number of wormholes and the distance in the log-log coordinate system. This indicates that vertical distribution of wormholes meets the fractal characteristics. Wormholes competition model explains how wormholes distribute.The calculation of the maximum wormhole length is the key step to solve this model, and with given steps, wormhole numbers of different length can be obtained.

On this basis, a dual-fractal model of wormhole distribution was established, which laid the foundation for the quantitative description of wormhole morphology in three-dimension and made the more accurate optimization of acidizing operation possible.

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1139

Using topology and energy balance to determine wettability in two and three-phase flow

Authors: Martin Blunt[1]; Takashi Akai[1]; Alessio Scanziani[1]; Qingyang Lin[1]; Abdulla Alhosani[1]; Branko Bijeljic[2]

[1] *Imperial College London*

[2] *Imperial College*

Corresponding Authors: alessio.scanziani16@imperial.ac.uk, q.lin11@imperial.ac.uk, b.bijeljic@imperial.ac.uk, t.akai17@imperial.ac.uk, m.blunt@imperial.ac.uk, abdulla.alhosani17@imperial.ac.uk

We use energy baance to determine contact angle. For three phases labelled 1, 2 and 3, assuming no change in Helmholtz free energy between two local equilibrium states and ignoring viscous dissipation $(\Delta a_{1s}\cos\theta_{12} - \Delta a_{12} - \phi\kappa_{12}\Delta S_1)\sigma_{12} = (\Delta a_{3s}\cos\theta_{23} + \Delta a_{23} - \phi\kappa_{23}\Delta S_3)\sigma_{23} + \Delta a_{13}\sigma_{13}$, where a is the interfacial area per unit volume, ϕ is the porosity, S is the saturation and κ the curvature of the fluid-fluid interface. The subscript s denotes the solid, and we consider changes, Δ, in saturation and area. The third contact angle, θ_{13} can be found using the Bartell-Osterhof relationship. The energy balance is also extended to an arbitrary number of phases.

We also propose a topological relationship: $2\pi n(1-\cos\theta) = 4\pi - \int \kappa_{G12}\, dS_{12}$ where n is the number of closed loops of the three-phase contact line where phases 1 and 2 contact the surface, θ is the average contact angle, while κ_{G12} is the Gaussian curvature of the fluid meniscus which is integrated over its surface S_{12}

With the advent of high-resolution three-dimensional X-ray imaging, the difference terms in the energy balance expression can be measured directly, while we can integrate curvature. This enables wettability, the contact angles, to be determined for complex displacements, to characterize the behaviour, and for input into pore-scale models.

Imaging datasets are used to illustrate the approach, comparing the flow of oil, water and gas in a water-wet and an altered-wettability carbonate sample. Using energy balance we show that in the water-wet case, as expected, water (phase 1) is the most wetting phase, oil (phase 2) is intermediate wet, while gas (phase 3) is most non-wetting with effective contact angles of $\theta_{12} = 48°$ and $\theta_{13} = 44°$, while $\theta_{23} = 0$ since oil is always present in spreading layers. In contrast, for the altered-wettability case, oil is most wetting, gas is intermediate-wet, while water is most non-wetting with contact angles of $\theta_{12} = 134°$, $\theta_{13} = 119°$, and $\theta_{go} = 66°$.

We also discuss the use of direct - geometric - and topological measures of wettability and how they complement the use of energy balance, allowing a rich and accurate characterization of wettability within porous materials.

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Investigation of adsorption and diffusion behaviors of multi-component gases in kerogen

Authors: Yu Shi[1]; Xiaona Yang[1]

[1] *Xi'an University of Science and Technology*

Corresponding Author: shiyu@xust.edu.cn

Multi-component gases are widely found in unconventional reservoirs such as coal rock, shale and tight sandstone. In this work, the adsorption and diffusion characteristics of multi-phase and multi-component gases in kerogen are studied based on the Molecular Dynamics method. It is shown that the adsorption capacity and diffusion coefficient of multi-component gases decrease with the increase of water. With the increase of temperature, the adsorption capacity of multi-component gases decreases whereas the diffusion increases. In contrast, with the increase of pressure, the adsorption capacity of multi-component gases increases while the diffusion decreases. Overall, the mechanism of transportation of multi-component gases in kerogen organic matter is revealed, which is usefulness for the efficient exploitation of unconventional gases.

Acknowledgments
This work was supported by the National Natural Science Foundation of China under Grant No. 11802231, the Natural Science Foundation of Shaanxi Provincial Department of Education under Grant No. 18JK0514, and the Natural Science Basic Research Program of Shaanxi Province under Grant No. 2019JQ-494.

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Optimizing carbon dioxide storage in oilfields at the pore-scale

Author: Abdulla Alhosani[1]

Co-authors: Qingyang Lin [1]; Alessio Scanziani [1]; Branko Bijeljic [2]; Martin Blunt [1]

[1] *Imperial College London*

[2] *Imperial College*

Corresponding Authors: b.bijeljic@imperial.ac.uk, q.lin11@imperial.ac.uk, m.blunt@imperial.ac.uk, abdulla.alhosani17@imperial.ac
alessio.scanziani16@imperial.ac.uk

We use X-ray imaging to investigate the mechanisms of CO2 storage in oilfields at immiscible and near-miscible CO2-oil injection conditions; at these conditions, three fluids phases exist inside the rock pore space: CO2, oil and water. We image trapped, residual, CO2 saturation in a reservoir rock with altered wettability (oil-wet) extracted from a giant producing oil reservoir in the Middle East. We adopt a water-CO2-water injection strategy, typical of enhanced oil recovery (EOR) projects, where CO2 storage is most economical. We compare the wettability order, pore occupancy, fluids connectivity and configuration, CO2 trapping mechanism, oil recovery, interfacial areas and capillary pressures at immiscible and near-miscible conditions and suggest the optimum injection strategy to optimize both CO2 storage and oil recovery at these conditions.

We observe that at both injection conditions, the wettability order in the system is altered such that water is the most non-wetting phase occupying the largest pores, oil is the most wetting phase occupying the smallest pores, while CO2 is the intermediate-wet phase occupying medium-sized pores. This wettability order, oil-gas-water from most to least wetting, was theoretically predicted but never experimentally reported. Nevertheless, despite having the same wettability order, we observed different pore-scale fluids configuration at immiscible and near-miscible conditions.

CO2 spreads in layers surrounding water at near-miscible conditions, while, at immiscible conditions, it exists as disconnected ganglia. Water gets trapped in the centres of the pore space when CO2 is injected at both conditions, with slightly higher water trapping at immiscible conditions. CO2 is more connected at near-miscible conditions, albeit with a low flow conductance. Oil exists in thick wetting layers close to the rock surface at both conditions. It is not possible to capillary trap CO2 by water in the centers of the pore space at both immiscible and near-miscible conditions since CO2 is more wetting to the rock than water. However, capillary trapping of CO2 by oil is possible at immiscible conditions only. The efficiency of oil recovery is much higher at near-miscible conditions due to the low gas-oil capillary pressure which gives a higher microscopic displacement efficiency.

Given the low flow conductance of CO2 and high CO2-oil displacement efficiency at near-miscible conditions, an injection strategy of continuous CO2 injection is suggested to optimize both oil recovery and CO2 storage. On the other hand, given the possible capillary trapping of CO2 by oil, highly disconnected CO2 phase, and the low CO2-oil displacement efficiency, an injection strategy of water-CO2-water is recommended at immiscible conditions.

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An experimental study on the impacts of gas pressure on carbon isotope fractionation during methane desorption in shale rock

Author: Yongbo Wei[1]

Co-authors: Shuangfang Lu ; Junqian Li ; Wenbiao Li

[1] *17806227064*

Corresponding Author: s19010075@s.upc.edu.cn

Methane carbon isotope fractionation during shale gas desorption provides a new approach to evaluating the gas in-place (GIP) content and the ratios of adsorbed and free gas as well as predicting the production status of shale gas wells (Li et al., 2020). However, it is unclear how the reservoir pressure (gas pressure), which is an important parameter in shale gas desorption, affects the methane carbon isotope fractionation. Considering anisotropic pressures in shale gas in-situ reservoirs, five gas pressure values (i.e., 2, 4, 6, 8, and 10 MPa) were selected for this study to perform methane isotherm

adsorption-desorption experiments for four shale samples from the Wufeng and Longmaxi Formations in the southeastern Sichuan Basin, and the characteristics of carbon isotope fractionation (CIF) during methane desorption processes were investigated. Results show that: (1) under different gas pressures, CIF of the in-methane transport process shows four stages: stable stage (free gas seepage stage) (I), lighter stage (transition stage) (II), heavier stage (adsorbed gas desorption stage) (III), and another lighter stage (concentration diffusion stage) (IV). The CIF law in shale gas migration under different gas pressures is consistent with the general isotope fractionation pattern during production by our previous study (Li et al., 2020), which shows that the model has certain guiding significance for shale gas reservoirs with varied buried depth/reservoir pressures; (2) CIF during methane desorption is impacted by multiple factors including the total organic carbon (TOC) content, pore structure, gas pressure, and adsorbed gas ratio, while material composition and pore structure largely determine the characteristics of isotopic fractionation in methane desorption, which are extremely important control factors; and (3) gas pressure has an obvious effect on CIF characteristics by changing the proportion of adsorbed gas, especially in stages II and IV, and the sample with developed organic matter had a stronger response. The higher the ratio of adsorbed gas, the larger the range of isotope fractionation. This demonstrates the significance of adsorption-desorption for CIF in shale gas migration.

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1143

Development of multi-physics models accounting for reversible flow at various subsurface energy storage sites

Author: Beatrix Becker[None]

Co-authors: Bernd Flemisch [1]; Rainer Helmig [1]; Bo Guo [2]; Karl Bandilla [3]; Mike Celia

[1] *University of Stuttgart*

[2] *University of Arizona*

[3] *Princeton University*

Corresponding Authors: beatrix.becker@iws.uni-stuttgart.de, rainer.helmig@iws.uni-stuttgart.de, bandilla@princeton.edu, bernd.flemisch@iws.uni-stuttgart.de, celia@princeton.edu

Simulating large scale underground energy storage for risk assessment and planning purpose requires simulations for multi-phase and multi-component flow on a large domain over the whole time of plant operation and beyond, including local features such as fault zones and a representation of the fluctuating gas plume front. In addition, often a large number of simulation runs need to be conducted to quantify parameter uncertainty. Efficient models are needed as well to integrate measurements during simulation to improve predictions (e.g. by means of data assimilation). Within acceptable computational time this cannot be achieved by full three-dimensional multiphase multicomponent models due to limited computational resources. Aim of this presentation is therefore to show an efficient multi-physics model to simulate underground energy storage. The model couples vertically integrated models with full-multidimensional models, including those processes relevant to an accurate solution while being computationally fast.

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1144

Proactive Optimization of CO2 Sequestration under Geomechanical Constraints

Author: Mohammad Salehian[1]

Co-author: Aliakabar Hassanpouryouzband [2]

[1] *Institute of GeoEnergy Engineering, Heriot-Watt University, UK*

[2] *School of Gesosciences, University of Edinburgh, UK*

Corresponding Authors: hssnpr@ed.ac.uk, ms315@hw.ac.uk

Development of a safe and economical Carbon Dioxide Capture and Sequestration (CCS) technology has caught significant attention in recent years. The possibility of long-term sequestration of CO2 in saline aquifers has been investigated by several studies. However, the detailed information regarding the optimal control and management of these processes has not been deeply addressed yet. This work addresses an integrated decision-making framework for long-term optimization of the CO2 sequestration, examining the trade-offs between the project profitability, efficiency of CO2 utilization, and reservoir stability. A kinetic model is integrated with a compositional thermal reservoir simulator, describing the reactive transport of CO2 in a 3D geological system. Residual and solubility trapping is considered within our developed model to account for CO2 precipitation in a mineralized form. A two-way geomechanical model has been incorporated into the model, in order to estimate the overall porosity and permeability changes in the field, affected by kinetic reactions and mineralization processes. Particle Swarm Optimization (PSO), a metaheuristic stochastic optimization algorithm, is applied to simultaneously optimize the short-term and long-term storage strategy by rearranging the injection scenario in multiple control steps. Results show that proactive optimization of CO2 sequestration processes can significantly improve the economics and long-term efficiency of a CCS project while reducing the risk of CO2 leakage due to geomechanical deformation. The presented workflow integrates critical challenges that are correlated, yet often addressed independently, supporting the complex decision-making of CO2 sequestration operational design in saline aquifers.

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Quantifying Uncertainty Reduction in Geologic CO2 Sequestration Risk Assessment

Authors: Bailian Chen[1]; Dylan Harp[1]; Rajesh Pawar[1]

[1] *Los Alamos National Laboratory*

Corresponding Author: bailianchen@lanl.gov

Geologic CO2 sequestration sites usually have large uncertainty in geological properties, such as uncertainty in permeability and porosity fields. Geological uncertainty leads to significant uncertainty in predicted risk quantities such as CO2 plume extent, CO2/brine leakage rates through wellbores, and impacts to drinking water quality in groundwater aquifers due to CO2/brine leakage, all of which will impact the approach for post injection site care (PISC). Pre-injection risk assessment can be used to quantify the amount of uncertainty in different predicted risk quantities. However, it cannot account for the potential value of monitoring data (e.g., CO2 saturation and pressure measurements) acquired during the operation of CO2 storage. In this presentation, we demonstrate how uncertainty in predicted quantities can be reduced by performing monitoring data assimilation.

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1148

Numerical Studies on Reactive Flow in Porous Media: An Example of Carbonate Matrix Acdizing

Authors: Cunqi Jia[None]; JUN YAO[1]

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

Corresponding Author: b17020093@s.upc.edu.cn

Matrix acidizing is widely used as a practical stimulation technique to improve matrix permeability. In this work, a new two-scale continuum model is used to study 2-D acidizing process, which uses Navier-Stokes-Darcy equation instead of Darcy equation to describe fluid flow and considers mass exchange between fluid and solid phases. Based on this model, a sensitivity analysis is presented to study effect of parameters including acid injection velocity, acid injection concentration, surface reaction rate, viscosity, core geometries, initial porosity, and medium heterogeneity.
The model can well capture optimum acid injection velocity and typical dissolution patterns observed in experimental studies. It is proved that the substitution of Navier-Stokes-Darcy equation for Darcy equation is correct and necessary because Darcy equation does not well capture physical behaviors of fluid phase in conical wormhole and face dissolution regions. As for effect of acid properties, decreasing injected acid concentration significantly increases amount of solute (usually water) but acid mass required to breakthrough doesn't change a lot. Optimum acid injection velocity and least PVTB are very sensitive to surface reaction rate. For example, strong acid can effectively reduce least PVTB but meanwhile optimum acid injection velocity is obviously increasing. Effect of viscosity is only obvious at low acid injection velocity. As for effect of rock properties, the increase of core length and diameter both results in more acid consumed. At high acid injection velocities, acid injection mass increases as initial porosity increases. At low acid injection velocities, however, the amount of acid decreases as initial porosity increases. Like viscosity, both porosity heterogeneity and permeability heterogeneity main affect conical wormhole and face dissolution regions.

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Bandwidth re-fracturing technique optimization and design consideration in naturally-fractured tight reservoirs — Case study on Ansai oil field, Ordos basin

Author: Xia Du[None]

Co-authors: YuLiang Su [1]; Wendong Wang [2]; Ning Zhao ; Dongsheng Li

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

[2] *School of Petroleum Engineering, China University of Petroleum (East China), 266580, Qingdao, China*

Corresponding Authors: lidongsheng_upc@163.com, suyulangupc@upc.edu.cn, zhaoningupc@gmail.com, duxia_upc@163.com

In high water-cut stage, tremendous remaining oil still accumulates as water floods along the high-permeability channels due to the existence of natural fractures in tight reservoirs. During re-fracturing, if the bandwidth is too large, water breakthrough would lead stimulation to failure. In this work, a methodology to design bandwidth of re-fracturing is implemented. The numerical models which take production induced stress field into consideration are established to obtain the optimal bandwidth of re-fracturing.
Based on elliptical seepage theory, the minimum bandwidth was designed to break through the primary drainage area calculated by threshold pressure gradient and stress sensitive constant to capture sufficient oil. A set of high-resolution 3D reservoir models are constructed to analyze the distribution of remaining oil based on the field data obtained from Ansai Oilfield, Ordos Basin. Then, take water-cut rising speed into consideration, the bandwidth with low final water-cut and maximum cumulative oil production is selected as the optimal maximum bandwidth.
Due to high threshold pressure gradient(0.43 MP/m) and low permeability(0.2mD), drainage radius of each well is pretty small, whereas re-fracturing could efficiently expand drainage area to obtain higher production according to simulation. It is observed that remaining oil accumulates surround lateral wells and low-permeability areas where streamlines are remarkable sparse. On the contrary, water breakthrough mostly happens in main wells. As bandwidth grows bigger, drainage area expands with an increase in production and water-cut, correspondingly. However, once the limitation is reached, secondary fractures would extend to water-flooded zone, and water would rush into wells, rarely sweeping remaining oil. Finally, a bandwidth with lower final water-cut and higher cumulative oil production underneath the limitation point was selected as the maximum bandwidth. Through sensitivity analysis, it is further observed that reservoirs with larger permeability always corresponds to smaller maximum bandwidth and larger minimum bandwidth, water-cut is higher of course. Therefore, customized bandwidth for each well with various permeability could impressively enhance the effect of stimulation.
The models established with production induced stress field could improve the accuracy of the optimal design effectively. And the typical chart presented in this work contains bandwidths suitable for reservoirs with different permeability. Theoretically, this methodology can be readily utilized in most high water-cut tight reservoirs with natural fractures. After applied in Ansai Oilfield, production increases 10%, with an increase in water-cut of 7% only, which proves the feasibility of our work.

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Dynamic synchrotron microtomography and pore-network modelling for direct in-situ capillary flow observation in 3D printed lab-on-chips

Authors: Agnese Piovesan[1]; Tim Van De Looverbosch[None]; Pieter Verboven[2]; Clement Achille[None]; Cesar Parra Cabrera[None]; Elodie Boller[None]; Yin Cheng[None]; Rob Ameloot[None]; Bart Nicolai[None]

[1] *KU Leuven*

[2] *KU Leuven - University of Leuven*

Corresponding Authors: pieter.verboven@kuleuven.be, agnese.piovesan@kuleuven.be

Capillarity driven lab-on-chips (LOC) are small, cheap devices capable of autonomously triggering fluid flow in functionalized porous channels. Such microfluidic channels, can nowadays be obtained through powder-based 3D printing 1. The pore microstructure and bulk material surface chemistry influence the microscale fluid dynamics, which in turn determines LOC performances.
Deep understanding and characterization of pore scale fluid flow are therefore essential to optimize capillarity driven LOCs. For this purpose, the dynamics of water imbibition in the LOC porous channels was visualized in-situ at the European Synchrotron Radiation Facility (ESRF) through fast X-Ray micro computed tomography (µCT). A 3D printed porous channel composed of unbound poly-methyl methacrylate (PMMA) powder was continuously imaged during water imbibition at the beamline ID19 of the ESRF, with space resolution of 1 µm and time resolution of 0.5s for a total of 12s. The reconstructed images at different time frames were subjected to post-processing in Avizo R1 (Visual Sciences Group, www.vsg3d.com) to segment the different phases (air, water and solid PMMA). The segmented images allowed us to follow water imbibition, as well as to compute the system effective contact angle in-situ. A preferential wicking direction was observed from the segmented images. The contact angle analysis suggested this to be caused by a variation of surface properties in the edge regions of the microfluidic channel. To test this hypothesis, a pore-network was built from the reconstructed geometry 2, on which spontaneous imbibition was dynamically modelled. Two different cases were modelled, one featuring constant surface properties of the porous matrix, and one considering the variation in contact angle observed from the in-situ measurements. Only the pore-network model with inhomogeneous surface properties was able to well reproduce the observed experimental behavior, indicating a varying contact angle to be the cause of the observed preferential wicking direction. This variation in surface properties was proved to be a consequence of fume generation taking place both during 3D printing (based on a dissolution-precipitation approach based on solvent inkjetting) and the following post-processing steps (drying and storage).
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Quantifying the Effect of Different Relative Permeability curves on Conventional and Unconventional Reservoirs during Natural and Enhanced Oil Recovery

Author: Isaac Obielum[1]

Co-authors: Paul Glover [1]; Piroska Lorinczi [2]

[1] *University of Leeds, UK*

[2] *University of Leeds*

Corresponding Authors: p.lorinczi@leeds.ac.uk, p.w.j.glover@leeds.ac.uk, obielumisaac@gmail.com

Understanding fluid flow in a heterogeneous and anisotropic reservoir even though it comes with its complexity has been an essential consideration for both geoscientists and engineers. A critical function in the flow and ultimate recovery estimations is the relative permeability, but the extent at which change in its curve shape influences the final output is unknown. The relative permeability curve used must be analyzed and modified before inputted into commercial simulators. Hence, the importance of pre-knowledge of reservoir properties like the pore distribution index, λ that determines the shape of the curve.

Extensive analysis was conducted using various experimental data from sandstones and tight oil reservoirs. These data were remodeled using fitting mathematical models to determine a spread of λ values providing different shapes of relative permeability curves. The method employed in characterizing the heterogeneity of the reservoir is the advanced fractal reservoir modeling (AFRM), designed using the concept of fractal geometry in determining irregularities of a 3D reservoir volume. Range of fractal dimensions, seed numbers, and anisotropic factors, outputted six different heterogeneous structures that are statistically enough for an individual rock type.

In a sandstone reservoir, the degree of heterogeneity and change in the relative permeability curve had little effect on the cumulative oil production for all structures, yielding a difference of ±5MMSTB at the end of simulated field life, although a higher λ value leads to lesser water production and longer water breakthrough time. This result is contrasting to that of the tight oil reservoir, whose ultimate recovery is mostly dependent on the shape of the relative permeability curve. Its reservoir production performance had a difference of 15% for every little change in the relative permeability curve for each simulated structure.

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Life in a tight spot: Bacterial motility in porous media

Authors: Tapomoy Bhattacharjee[1]; Daniel Amchin[1]; Jenna Ott[1]; Felix Kratz[1]; Sujit Datta[1]

[1] *Princeton University*

Corresponding Author: ssdatta@princeton.edu

Diverse processes in healthcare, agriculture, and the environment rely on bacterial motility in porous media; indeed, most bacterial habitats—e.g. biological gels, tissues, soils, and sediments—are heterogeneous porous media. However, while bacterial motility is well-studied in homogeneous environments, how confinement in a porous environment impacts bacterial transport remains poorly understood. To address this gap in knowledge, we combine microscopy, materials fabrication, and microbiology to investigate how *E. coli* moves in 3D porous media. By probing single cells, we demonstrate that the paradigm of run-and-tumble motility is dramatically altered by pore-scale confinement. Instead, we find a new mode of motility in which cells are intermittently and transiently trapped as they navigate the pore space; analysis of these dynamics enables prediction of bacterial transport over large length and time scales. Further, by developing a new 3D printing approach, we design multi-cellular communities with precise control over the spatial distribution of bacteria. Using this approach, we show that concentrated populations can collectively migrate through a

porous medium—despite being strongly confined—and develop principles to predict and direct this behavior.

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Bistability in the unstable flow of polymer solutions through porous media

Authors: Christopher Browne[1]; Audrey Shih[1]; Sujit Datta[1]

[1] *Princeton University*

Corresponding Author: ssdatta@princeton.edu

Polymer solutions are often injected in porous media for applications such as oil recovery and groundwater remediation. As the fluid navigates the tortuous pore space, elastic stresses build up, causing the flow to become unstable at sufficiently large injection rates. However, it is poorly understood how the spatial and temporal characteristics of this unstable flow depend on pore space geometry, which can vary widely between different porous media. We investigate this dependence by systematically varying the spacing between pore constrictions in a one-dimensional ordered array. We find that when the pore spacing is large, unstable eddies form upstream of each constriction, similar to observations of an isolated constriction. By contrast, when the pore spacing is sufficiently small, the flow in the different pores exhibits a surprising bistability, stochastically switching between two distinct unstable flow states. We hypothesize that this unusual behaviour arises from the interplay between elongation and relaxation of polymers as they are advected through the pore space. Consistent with this idea, we find that the flow state in a given pore persists for long times; moreover, flow states are strongly correlated between neighbouring pores. Thus, the characteristics of unstable flow are not determined just by injection conditions and the geometry of the individual pores, but also depend on the spacing between pores. Ultimately, these results help to elucidate the rich array of behaviours that can arise in polymer solution flow through porous media.

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Evaporation and condensation of water in nanopores with salt

Authors: Olivier Vincent[1]; Piyush Jain[2]; Marine Poizat[3]; Léo Martin[3]; Abraham Stroock[2]

[1] *CNRS*

[2] *Cornell University*

[3] *CNRS & Univ. Lyon 1*

Corresponding Author: olivier.vincent@univ-lyon1.fr

We studied evaporation and condensation of water in nanoporous media containing salt solutions. This situation is important in various contexts in nature and technology, e.g. geophysics, heritage

conservation, water harvesting etc. Our results show that the presence of salt dramatically modifies water sorption isotherms in a predictable manner, due to the combination of osmotic and surface tension effects. They also suggest that crystallization and deliquescence of the salts are strongly modified by confinement.

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Jain, P., Vincent, O. & Stroock, A. D. Adsorption, Desorption, and Crystallization of Aqueous Solutions in Nanopores. Langmuir 35, 3949–3962 (2019).

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Equilibria, kinetics, constraints, and multiple scales

Authors: Malgorzata Peszynska[1]; Choah Shin[2]

[1] *Oregon State University and National Science Foundation*

[2] *Oregon State University*

Corresponding Authors: shinc@oregonstate.edu, mpesz@math.oregonstate.edu

This talk contributes to the celebration of Rainer Helmig's Lifetime Achievement Award and will feature some results on computations with multiphase multicomponent models which have been central to Rainer's work.

Reservoir simulation models describe flow and transport coupled to other processes such as energy conservation and deformation, and these couplings have particular characteristic time and spatial scales associated with them. Handling these scales efficiently requires making assumptions. A particular example is of thermodynamic phase behavior which one can argue is always out of equilibrium, with equilibria approximating the kinetics at long time scales. In turn, one could argue that kinetic models can serve as efficient pseudo-transient solvers for the phase equilibria which they approximate.

In the talk we present our recent analyses and computations with equilibrium and kinetic models, focusing on methane transport and methane hydrate evolution in two phase conditions. We present three kinetics models and an equilibrium model which they approximate. Model 1 is well known in geochemistry and its extension is widely used in reservoir simulation including Rainer's work, but is nonlinear. Model 2 is linear and can be made equivalent to Model 1, under assumption of variable rate. However, both Model 1 and Model 2 work only well in saturated conditions. The new model we propose, Model 3, works across a wide range pf physically meaningful unsaturated and saturated conditions, thus is most robust when external thermodynamic controls change, while its solutions can be found with explicit algebraic expressions. The theory we develop is based on mathematical treatment of evolution problems with constraints, and we are able to prove stability of a finite volume scheme.

We hope to extend the theory further to the wide range of conditions that contain computational models developed by Professor Helmig and his collaborators.

If time allows we will include considerations of computations at the interface scale, i.e., below the pore-scale, of these processes, and how they connect to Darcy scale kinetics and equilibria.

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Real-time imaging reveals distinct pore scale dynamics during transient and equilibrium subsurface multiphase flow

Author: Catherine Spurin[1]

Co-authors: Sam Krevor ; Martin Blunt [1]; Steffen Berg [2]; Gaetano Garfi [1]; Maja Ruecker [1]; Tom Bultreys [3]; Vladimir Novak [4]; Christian Schleputz [4]

[1] *Imperial College London*

[2] *Shell Global Solutions International B.V.*

[3] *Ghent University*

[4] *Paul Scherrer Institute*

Corresponding Authors: m.blunt@imperial.ac.uk, tom.bultreys@ugent.be, steffen.berg@shell.com, cls13@ic.ac.uk, g.garfi17@imperial.ac.uk, s.krevor@imperial.ac.uk, m.rucker15@imperial.ac.uk

Many subsurface fluid flows, including the storage of CO_2 underground or the production of oil, are transient processes incorporating multiple fluid phases. The fluids are not in equilibrium meaning macroscopic properties such as fluid saturation and pressure vary in space and time. However, these flows are traditionally modelled with equilibrium (or steady-state) flow properties, under the assumption that the pore scale fluid dynamics are equivalent. In this work, we used fast synchrotron X-ray tomography with $1s$ time resolution to image the pore scale fluid dynamics as the macroscopic flow transitioned to steady-state. For nitrogen gas or a mineral oil, and brine injected simultaneously into a porous rock we observed distinct pore scale fluid dynamics during transient flow. Transient flow was found to be characterised by intermittent fluid occupancy, whereby fluid-fluid interfaces, and flow pathways through the pore space, were constantly rearranging. The intermittent fluid occupancy was largest and most frequent when a fluid initially invaded the rock. But as the fluids established an equilibrium the dynamics decreased to either static interfaces between the fluids or small-scale intermittent flow pathways, depending on the capillary number and viscosity ratio. If the fluids were perturbed after an equilibrium was established, by changing the flow rate, the transition to a new equilibrium was quicker than the initial transition. Our observations suggest that transient subsurface flows require separate modelling parameters from steady-state flows, especially for the initial invasion of a fluid. The timescales required to achieve equilibrium suggest that several metres of an invading CO_2 plume front will have flow properties controlled by transient pore scale fluid dynamics.

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Molecular Simulation Study of Inorganic and Organic Porous Materials

Authors: Arun Kumar Narayanan Nair[1]; Shuyu Sun[2]

[1] *King Abdullah University of Science and Technology (KAUST), Saudi Arabia*

[2] *King Abdullah University of Science and Technology (KAUST)*

Corresponding Authors: shuyu.sun@kaust.edu.sa, arun.narayanannair@kaust.edu.sa

Shale is a sedimentary rock rich in organic matter (such as kerogen) and inorganic constituents (such as clay minerals). Ten years into the shale revolution, thanks to the advancement in the fracking technology, shale gas has drastically changed the game of energy in the world. Furthermore, the

usage of anthropogenic carbon dioxide for the extraction of oil and gas from shale reservoirs provides a unique way to reduce emissions. In this work, molecular simulations were performed to understand the mechanisms of gas sorption and transport in both inorganic (clays) and organic (carbon nanotubes) materials. Our results confirm the experimental observation that the high-charge clays generally shift swelling transition towards lower relative humidity values. Also, our results show that in inorganic pores, the adsorption selectivity of carbon dioxide over methane decreases with pressure in dry condition, however, this trend is reversed in the presence of water. Both in the organic and inorganic pores, the presence of carbon dioxide significantly affects the mobility of methane.

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Simulation of two-phase flow in fractured media with discontinuous capillary pressure

Author: Luat Khoa Tran[None]

Co-author: Stephan Matthai [1]

[1] *The University of Melbourne*

Corresponding Authors: stephan.matthai@unimelb.edu.au, luatkhoat@student.unimelb.edu.au

In fractured porous media, the abrupt changes on physical quantities at fractures - matrix interface yield profound effects on the two-phase flow pattern. These local discontinuities cause difficulties for both spatial discretization and realistic flow simulation. We develop a new vertex-centred finite volume scheme which provides a sufficient degree of freedom to correctly discretize the geological domains and describe jump discontinuity of flow variables. Furthermore, the computed saturation values at the fracture-matrix interfaces are always satisfying Van Duijn-De Neef condition.
We demonstrate the effectiveness of the method on a variety of test case including gravity, capillary pressure and material discontinuities.

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4-D Imaging of Desaturation of the Frozen Gas Diffusion Layers by Synchrotron X-ray Radiography

Author: Zhang Yuzhou[None]

Co-authors: Viral Hirpara ; Virat Patel ; Ryan Anderson ; Ning Zhu ; Lifeng Zhang

Corresponding Authors: lifeng.zhang@usask.ca, yuz097@mail.usask.ca

The 4-D analysis of the thawing and desaturation process of the initially saturated, frozen gas diffusion layer (GDL) with a serpentine gas flow channel was performed based on the synchrotron X-ray tomography images. High speed and rapid CT scanning during the experiments allowed the

research on the dynamic desaturation under the cold start-up and gas purging condition. The saturation profile was studied over then entire GDL domain, through the vertical plane, and in the selected region for localized behaviors. Sigracet 35AA and 35BA GDLs were selected for the experiments to study the effects of material hydrophobicity. The average desaturation rates over the entire purging process were 0.000186 μL cm^{-2} s^{-1}, 0.000470 μL cm^{-2} s^{-1}, 0.000516 μL cm^{-2} s^{-1} and 0.000901 μL cm^{-2} s^{-1} for the superficial gas velocity of the purging air at 2.88 m/s, 4.26 m/s, 5.98 m/s and 9.02 m/s, respectively. In addition, the dynamic 3-D models were constructed to show the liquid water movement through a GDL in the interested area. Although the GDL desaturation curves for each experiment shared the similar trend, our results showed that different conditions including initial saturation, air flow rate, GDL material properties could affect both overall and local desaturation behavior. These data could provide valuable information for the future modeling studies that involve the thawing process in the GDL/channel region; and could be used to optimize the cell design and develop cold start-up protocols.
Keywords: PEM fuel cell, gas diffusion layer, cold start-up, saturation, X-ray radiography, 4-D imaging

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Modeling the droplet occurrence, growth and detachment at the interface between the porous layers in a PEM fuel cell coupling a pore-network model with Stokes flow

Author: Cynthia Michalkowski[None]

Co-authors: Maziar Veyskarami ; Carina Bringedal ; Rainer Helmig [1]

[1] *University of Stuttgart*

Corresponding Authors: cynthia.michalkowski@de.bosch.com, rainer.helmig@iws.uni-stuttgart.de, maziar.veyskarami@iws.uni-stuttgart.de, carina.bringedal@iws.uni-stuttgart.de

For improved operating conditions of a polymer electrolyte membrane fuel cell (PEM FC), a sophisticated water management is crucial. Therefore, it is necessary to understand the transport mechanisms of water throughout the cell constituents especially on the cathode side, where the excess water has to be removed. Microscale modeling of diffusion layers and gas distributor has been established as a favorable technique to investigate the ongoing processes.
Investigating the interface between the cathode layers, a particular challenge is the combination and interaction of the multiphase flow in porous material of the GDL with the free flow in the gas distributor channels. The formation, growth and detachment of droplet on the hydrophobic, porous surface has a major influence on the mass, momentum and energy exchange between the layers.
To capture the droplet occurrence and its influence on the flow, a dynamic two-phase pore network model is coupled with a free flow gas channel model fulfilling the mass, momentum and energy balance.
Based on a macroscopic force balance analysis in a three-dimensional domain, an analytical solution in terms of dynamic contact angle and gas flow velocity in the channel is obtained for the detachment of droplets in steady, fully developed flow.
The droplet occurrence and growth results explicitly from the multi-phase multi-component flow in the pore network and modelled using dynamic coupling conditions for the mass, momentum and energy exchange between the domains.
The model is able to represent the dynamic interaction of the porous GDL and the gas distributor flow including the mutual interaction of droplet formation, growth and detachment.

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Pore and Permeability Modeling Research of the CO2-bearing Strata in Wuerxun Depression

Authors: mingyue lu[1]; Ning Qi[2]

[1] *17686433563*

[2] *17806278642*

Corresponding Authors: 1430067486@qq.com, 49142456@qq.com

In this paper, through theoretical data and three-dimensional geological modeling, the geological conditions of the Wuerxun Depression in the Surennuoer area are studied and analyzed. Verification of the existing logging data in the study area confirmed the fidelity of the model. The magma enrichment in the Suren Nuoer area of the Wuerxun depression and the control of deep and large fault basins make it possible for CO2 to have sufficient gas sources and advantageous migration channels, which has become one of the conditions for CO2 enrichment in the Suren Nuoer area. The carbon dioxide in the study area is mainly due to the magma-volcanic source in the inorganic origin. By establishing a grid model of pore permeability and analyzing the physical property data, the southern section of the study area has better physical properties, and the volcanic rock pore permeability is better than ordinary sandstone than lamellar sodium aluminum Stone sandstone, and the dawsonite sandstone layers in the study area are mostly adjacent to the carbon dioxide-containing layers. In this paper, this phenomenon and the physical properties of the southern section of the study area will be studied to provide optimal horizon support for carbon dioxide capture in the study area

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Research on geological modeling of porosity and permeability in CO2 gas reservoirs——Taking Surennuor area as an example

Authors: Ning Qi[1]; Mingyue Lu[2]

[1] *17806278642*

[2] *17686433563*

Corresponding Authors: 49142456@qq.com, 1430067486@qq.com

In order to more intuitively and accurately reveal the three-dimensional spatial distribution of carbon dioxide gas reservoirs in the Surennuoer Oilfield in the Hailar Basin, the author integrated data such as core, seismic, well logging, drilling, and production performance to constrain and finely construct the south of the Surennuoer gas field. The three-dimensional effective thickness, deep and large fault system, porosity, permeability, water saturation distribution model of the Tun Formation and Tongbomiao Formation, comprehensive geological modeling studies have found that the region has the following characteristics: ① CO2 gas reservoirs are mainly distributed in the low pores of the southern section In the low-permeability sandstone reservoirs, a small amount is distributed in the

middle-low porosity and low-permeability sandstone reservoirs in the second member of the South; ② There is a set of tens of meters of mudstone caprock between the second member of the South and the first member of the South, which blocks the CO2 gas reservoir in the South ; ③ The widely distributed mudstones of the Damaoguai Formation can be used as regional caps to block the lower CO2 gas reservoir. ④The carbon dioxide gas reservoir of Nantun Formation is a gas reservoir with low permeability, low porosity and extremely developed faults. It provides a basis for solving the problems of favorable exploration areas and predicted reserves of carbon dioxide gas reservoirs, and provides a data body for the formulation of later development plans.

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Direct pore scale simulation of water in nanoporous shale and prediction of apparent liquid permeability

Authors: Tao Zhang[1]; Ying Yin[2]; Xiangfang Li[3]

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

[2] *Xi'an Jiaotong University*

[3] *China University of Petroleum*

Corresponding Author: tobiascheuing@163.com

Water flow in nanoporous structures in shale strongly depends on water-pore wall interactions. Because of strong water-pore wall interactions, the models that govern flow in nanoporous structures deviate from conventional continuum flow models such as the Darcy equation.
First, a lattice Boltzmann method (LBM) with nanoscale physics embedded for nanoconfined water flow is established by using mesoscopic forces to capture the water-solid interactions. The simulation results of the proposed model are in good agreement with the majority of 48 different cases of flow in single nanotube with different materials and dimensions in the literatures. Second, the stochastic 3D nanopore systems of organic matter (OM) is reconstructed and constrained by comparing pore size/shape distribution of 2D high-resolution scanning electron microscope (SEM) images. Finally, by the LBM, the water flow in the reconstructed nanoporous media are simulated.
The most significant finding is that the contraction/expansion effects of pore-throat-pore systems in nanoporous OM weaken the hydrophobicity-induced slippage effect on total water flow, although the water transport capability in single hydrophobic nanotube, dependent on its wettability, is greatly enhanced compared with that predicted by the classical no-slip Poiseuille equation.
The work also highlights the importance of the accuracy of reconstructed 3-D pore networks in terms of pore connectivity, shape, and tortuosity in individual systems of OM. The proposed framework opens up a new avenue for modeling the water flow in experimental accessible and geometrically complex nanoporous media (eg. shale) with high computation efficiency, but achieving similar accuracy of molecular dynamics (MD) simulations.

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Optimization of fracturing parameters in shale gas reservoir by a

modified variable-length particle swarm optimization algorithm

Author: Zhihao Li[None]

Co-author: Jun Yao [1]

[1] *Research Center of Multiphase Flow in Porous Media*

Corresponding Author: lizhihao_upc@163.com

Horizontal drilling and hydraulic fracturing are recognised as the most effcient stimulation technique to enhance recovery in shale gas reservoirs, while little work has been done on fracturing parameters optimization. The flow mechanism in shale reservoir is complex due to the low permeability and thus it is imperative to optimize the substantial fracturing parameters economically under the current low price of natural gas. Optimization of fracturing parameters is regarded as a typical variable dimension varying problem when considering the property difference of fractures. Assuming that each fracture has three properties, half-length, conductivity and bifurcate angel. The increment of each additional fracture will introduce three extra variables. Conventional optimization of fracturing parameters was implemented by heuristic algorithms such as genetic algorithm (GA) and particle swarm optimization algorithm (PSO), however, with poor performance when dealing with problems that variable dimension varies during iteration. Thus an improved algorithm named modified variable-length particle swarm optimization (MVPSO) was proposed and verified by several classification problems from UCI machine repository in order to automatically select the optimal number of fractures as well as corresponding half-length, coductivity and bifurcate angel for maximizing the net present value (NPV). Fractures were simulated by the embedded discrete fracture model (EDFM) and fracture network was generated based on fractal methods. Results obtained indicated that the hydralic fractures performed in an irregular way and multi-spindle shaped instead of the homogeneous distribution. Besides, considerable increase in NPV can be realized by using MVPSO to obtain the optimal fracturing parameters in heterogeneous formation. The proposed algorithm is suitable to solve such dimension varying problems, before which seldom research was implemented.

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EUTROFICATION CONTROL TREATMENTS AND CARBON GAS EMISSIONS

Authors: DAngelo A. Sandoval[1]; Anne M. Hansen[2]; Armando González-Sánchez[3]; Rodolfo Sosa-Echeverría[4]

[1] *Graduate Program of Environmental Engineering, National Autonomous University of Mexico (UNAM)*

[2] *Mexican Institute of Water Technology (IMTA)*

[3] *Institute of Engineering, UNAM*

[4] *Center for Atmospheric Sciences, UNAM*

Corresponding Authors: ahansen@tlaloc.imta.mx, rodsosa@unam.mx, dangelo.sandoval@gmail.com, agonzalezs@iingen.unam.mx

Fresh water bodies emit 3.9 e+15 g yr-1 of carbon gases corresponding to 4% of total emissions 1. In Mexico 70% of the water bodies are eutrophied 2, and therefore they absorb and emit important amounts of carbon gases through photosynthesis and respiration processes. Part of the absorbed carbon is accumulated as organic matter in water and porous sedimentary material, where biodegradation processes of bioavailable organic matter cause carbon gas emmissions. Carbon accumulated

in smaller pores are usually not available for biodegradation. To control eutrophication of water bodies, the application of control technologies are urgently requiered and for this purpose, hypolimnetic oxygenation (HOS) and application of Phoslock (PHOS) that irreversibly adsorbs phosphorus, have proven to be efficient technologies 3. The objective of this study was to evaluate the effects of HOS and PHOS on carbon gas emissions from sediments in a eutrohied reservoir. The following treatments were applied to water and porous sediment samples incubated in reactors: HOS, PHOS, HOS+PHOS, and No Treatment (NT), and redox potential (Eh) and carbon gas emmissions were monitored during seven months. Nutrients were added regularly starting in month 4 to stimulate biodegradation in the reactors. Observed CO2 emission rates were HOS (112)>HOS+PHOS (89)>NT (12)>PHOS (6 mmol m-2 d-1), all values higher than reported for eutrophied water [4]. CH4 emission rates were: NT (48)>PHOS 13)>HOS+PHOS (2)>HOS (0.8 mmol m-2 d-1), with values for HOS and HOS+PHOS within those reported for mesotrophic water, while for the PHOS treatment and the NT, emissions were higher than reported in the literature [4]. It was observed that in the NT reactor, biodegradation occurred at different redox potentials, between -300 and 300 mV, PHOS caused biodegradation to mainly occur between -250 and -150 mV, while both reactors where oxygen was being added, occurred between -250 and -200 mV. Amounts of carbon gas emmitted was associated to organic carbon contents in untreated and treated sediment samples. Amounts of remaining organic carbon was related to the porous structure of the sediments. The financial supports from IMTA (TH1913.1 and TH2012.1), Conacyt (scholarship- CVU 780094) and the Office of International Affairs and External Cooperation of the University of Costa Rica, are acknowledged.

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Various Mathematical Approaches to Mechanical Simulations in Wound Healing Processes

Authors: Qiyao Peng[1]; Fred Vermolen[1]

[1] *Delft University of Technology*

Corresponding Authors: f.j.vermolen@tudelft.nl, q.peng-1@tudelft.nl

Deep tissue injury often results in contraction of skin due to mechanical pulling forces exerted by skin cells in the dermal layer. If contractions are morbid, then they are referred to as contractures. Contractures cause disabilities to the patients, by, for instance, loss of mobility of a joint. By the use of modeling, we aim at understanding the mechanisms behind the formation of a contracture and at predicting which wound is likely to develop a contracture and which treatments can be employed to minimize the likelihood of a contracture. Since the cells are much smaller than the domain of computation, we used the immerse boundary approach based on a superposition of Dirac Delta functions to describe the forces exerted by individual skin cells. The use of this superposition of Delta functions results in a numerical solution that is not in H1. Hence, other alternative approaches are developed to avoid it.

In particular, to describe contractions during wound healing, the forces exerted by cells are actually applied on a continuous curve. Therefore, the region covered by the cell is modelled as a hole in the domain, then the surface forces at the cell are formulated by means of a force boundary condition. The last-mentioned approach shows consistency with the immersed boundary approach, which is proved both analytically and numerically. All the simulations and results will eventually contribute to modelling the contractions of the wound.

On the other hand, we are hunting for the approaches in a general perspective which entail smoothed Dirac Delta distributions. Additionally, we also analyzed a homogenization approach based on Green's fundamental functions. A Gaussian regularization is widely used as a replacement of Dirac Delta distribution. In this approach, the selection of the variance has a significant influence on the solution. For one dimension, it is relatively straightforward to demonstrate convergence of the Gaussian distribution approach to the solution using Dirac Delta distribution as the variance is decreasing.

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Local and global sensitivity analysis of THM consolidation around a point heat source

Author: Aqeel Afzal Chaudhry[1]

Co-authors: Jörg Buchwald [2]; Thomas Nagel [3]

[1] *Technische Universität Bergakademie Freiberg, Germany*

[2] *Helmholtz Centre for Environmental Research –UFZ*

[3] *Technische Universität Bergakademie Freiberg*

Corresponding Authors: thomas.nagel@ifgt.tu-freiberg.de, joerg.buchwald@ufz.de, aqeel.chaudhry@ifgt.tu-freiberg.de

Coupled thermo-hydro-mechanical (THM) models are used for the assessment of nuclear waste disposal, reservoir engineering and geotechnical engineering. Model-based decision making and optimization require sensitivity analyses (SA) and uncertainty quantification (UQ). Assessment of different UQ and SA methods that work for coupled THM problems on an engineering scale is required. Due to different coupling levels, non-linearities, and large system sizes these analyses can be challenging. For an initial screening, it is advantageous to have an analytical solution that encompasses the most relevant primary couplings, can robustly cover the entire parameter space and remains computationally inexpensive.

Booker and Savvidou (1985) and Chaudhry et al. (2019) provided such an analytical solution for consolidation around a point heat source. We compared the different approaches to sensitivity analyses: local (OVAT) and global sensitivity analysis (GSA) based on Sobol indices for different spatio-temporal settings to observe near and far-field effects as well as early- and late-stage system response. We show parameters and interactions that control the results in these different domains and provide physical interpretations. We provide application-oriented conclusions on the conditions which should be met when applying the different methods and examples for possible misinterpretations. The analysis can serve as a benchmark for UQ and SA software designed around numerical THM simulators.

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Precipitation and dissolution in complex media: modelling, upscaling and simulation

Authors: Carina Bringedal[None]; Florin Adrian Radu[1]; Iuliu Sorin Pop[2]; Lars von Wolff[3]; Manuela Bastidas[2]

[1] *University of Bergen, Norway*

[2] *Hasselt University*

[3] *University of Stuttgart*

Corresponding Authors: florin.radu@uib.no, manuela.bastidas@uhasselt.be, carina.bringedal@iws.uni-stuttgart.de, lars.von-wolff@mathematik.uni-stuttgart.de, sorin.pop@uhasselt.be

Processes of highest societal relevance like soil salinization or the production of geothermal energy, involve precipitation and dissolution processes in porous media. Of particular interest is the situation when such processes lead to changes at the scale of pores, affecting Darcy scale properties like the medium porosity or its permeability.
In this talk we discuss different approaches for modelling precipitation and dissolution in porous media. Starting with models defined at the scale of pores, we employ homogenization techniques to derive models that are valid at the Darcy-scale, thus better suited for numerical simulations. After this we discuss different aspects related to the numerical algorithms.

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Investigating the effect of SIO2 nano particles on interfacial tension as EOR indicator

Author: ALI ALSAFFAR[None]

Co-author: abbas Abubakar [1]

[1] *University of Salford*

Corresponding Authors: a.i.a.alsaffar@edu.salford.ac.uk, a.j.abbas@salford.ac.uk

As many oil fields approaches final stages of production, new technologies are necessary to maximize the recovery of remaining hydrocarbons.Recently, techniques (EOR) using injection of Nano fluids (nano particles suspension) has become an attractive method that can potentially improve the effectiveness of the conventional water flooding approach .Researchers have introduced new methods for (EOR) and hence satisfy the growing demand for hydrocarbons . Recent advances in the field of nanotechnology means low cost nano particles can be produced at industrial scale and this allows planning and implementation of efficient and environmentally friendly methods of EOR .

This study investigates the effect of Nano particles on the inter facial tension using pendant drop technique, which could highlight the compatibility of nano-particles in the displacement of untapped hydrocarbons for enhance oil recovery. Hydrophilic silica dispersed in (i) brine, and (ii) distilled water were used with particles concentrations of 0.1, 0.2, 0.3 wt%. The inter facial tension IFT, of oil/nano fluids system was measured in order to assist in explaining the underlying mechanism behind the increased recovery. The inter facial tension measurements were performed at four temperature ranges, 25,50,75 and 100° C to simulate the reservoir conditions. In total, two series of inter facial tension measurements were performed using the pendant drop .
The measurements showed that Nano fluids have the ability to reduce the inter facial tension depending on the dispersion fluid, temperature, and Nano fluid concentration. The highest reduction was observed at 50° C, when Nano fluids with 0.1 wt % concentration, dispersed in 1 wt% brine were used . The inter facial tension decreased from 32.1 mN/m to 5.57 mN/m. However, the same value of inter facial tension increased to 29.09 mN/m at 100° C. On the other hand, Nano particles dispersed on distilled water showed less reduction on the inter facial tension. The highest reduction was seen at 75° C when 0.3 wt % Nano fluids concentration were used. The inter facial tension decreased from 36.2 mN/m to 14.07 mN/m.

The reduction of the inter facial tension when brine based Nano particles were used is resulted from the adsorption of Nano particles on the interface between oil and brine to replace the previous ones, therefore, the friction force of the two phases was reduced and hence generated lower IFT. If the reduction is large enough, more oil will be mobilized due to overcoming the capillary forces and minimizing the work of deformation required for oil droplets to move through pore throats.

Findings from this study has provided a potential for the use of this particular Nano particles in EOR and the following highlights :

- Nano fluids could reduce the inter facial tension depending on the dispersion fluid, temperature, and Nano fluid concentration.
- The highest reduction was observed at 50° C, when Nano fluids with 0.1 wt % concentration, dispersed in 1 wt% brine were used.
- Nano particles dispersed on distilled water showed less reduction on the inter facial tension.

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Effects of pore-size disorder on forced imbibition in porous media

Author: Lianwei Xiao[1]

Co-authors: Guangpu Zhu ; Jun Yao [2]

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

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

Corresponding Authors: yaojun@upc.edu.cn, s18020047@s.upc.edu.cn, zhugpupc@gmail.com

Imbibition, the wetting fluid displacing a nonwetting one, occurs in many natural and industrial applications, such as enhanced oil recovery and CO2 sequestration. The imbibition process is highly affected by the wettability conditions, viscosity ratio and injection flow rates, and the competition between these factors become more complicated when the disorder of pore-size effects is involved. In this work, we systematically investigate forced imbibition in five 2D porous media models with different disorder numbers over a broad range of wettability conditions and flow rates. We analyze

the relationship between interfacial length and the invading fluid saturation , and the relationship between displacement front and the invading fluid saturation . Results show that higher disorder of porous media can destabilize the displacement pattern. At the low capillary number, increasing the disorder leads the pattern shifting from stable displacement to capillary fingering. At the intermediate capillary number, increasing the disorder leads to larger interfacial area and lower displacement efficiency. At the high capillary number, increasing the disorder not only results in more chaotic viscous fingering with more tortuous fingers, but also decreases the critical capillary number , which corresponds to the cross-over from capillary-dominated regime to viscous-dominated regime. The phase diagrams based on different disorder number are presented, reflecting the disorder impact on imbibition process directly.
Keywords: imbibition; pore-size disorder; wettability; capillary number; porous media

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An accelerated staggered solution scheme to phase-field modeling of brittle fracture

Author: Erlend Storvik[1]

Co-authors: Jakub Both [1]; Juan Michael Sargado [2]; Jan Martin Nordbotten [1]; Florin Adrian Radu [3]

[1] *University of Bergen*

[2] *NORCE - Norwegian Research Centre AS*

[3] *University of Bergen, Norway*

Corresponding Authors: jakub.both@uib.no, jan.nordbotten@math.uib.no, jusa@norceresearch.no, erlend.storvik@gmail.com, florin.radu@uib.no

There is currently an increasing interest in enhancing the solvers applied to phase-field modeling of brittle fracture, see e.g., [1, 2, 3]. The governing equations for this problem originate from a constrained minimization of a non-convex energy functional, and the most commonly used solver is an alternate minimization scheme. This is known to be robust compared to the monolithic Newton method, however, alternate minimization often requires many iterations to converge when the crack is evolving. The focus of our work is to accelerate the solver through a scheme that combines Anderson acceleration and over-relaxation. This combined acceleration scheme takes advantage of the complementary strengths of Anderson acceleration and over-relaxation to make a robust and highly accelerating method for this problem. Moreover, the combined acceleration method is applied as a post-process, so the implementation can be done on top of already available code, and the activation of the scheme has a negligible cost. We present a numerical study, including well-known benchmark problems, that demonstrates the efficiency, and robustness of the method.

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2 P. Farrell, C. Maurini. Linear and nonlinear solvers for variational phase-field models of brittle fracture, Int. J. Numer. Meth. Engng. 109(2017). 648-667.

3 M.K. Brun, T. Wick, I. Berre, J.M. Nordbotten, F.A. Radu. An iterative staggered scheme for phase field brittle fracture propagation with stabilizing parameters, Comput. Methods Appl. Mech. Eng. 361(2020), 112752.

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Upscaled equations for two-phase flow in highly heterogeneous porous media

Author: Tufan Ghosh[1]

Co-authors: Carina Bringedal ; Rainer Helmig [2]; G. P. Raja Sekhar [3]

[1] *Institute for Modelling Hydraulic and Environmental Systems (IWS) University of Stuttgart*

[2] *University of Stuttgart*

[3] *Department of Mathematics, Indian Institute of Technology Kharagpur*

Corresponding Authors: rajas@iitkgp.ac.in, carina.bringedal@iws.uni-stuttgart.de, rainer.helmig@iws.uni-stuttgart.de, tufan.ghosh@iws.uni-stuttgart.de

In this study, we consider a two-phase flow model in a highly heterogeneous porous column. The porous column consists of homogeneous blocks, where the porosity and permeability vary from one block to the other. The flow direction is perpendicular to the layering of the porous column, and hence can be approximated by one-dimensional model equations. The periodic change in porosity and absolute permeability enforce the fluid to be trapped at the interface between the blocks, leading to a highly varying saturation. In order to capture the effective behavior, upscaled equations for the average saturation are derived via homogenization. This technique relies on a notion of periodicity and allows averaging over any number of blocks that may have any internal distributions of the rock parameters. Moreover, the present study also derives effective equations for randomly distributed layers of different porosity and absolute permeability. Numerical experiments are performed which show good agreement between the averaged solutions of the original micro-scale equations and the solutions of the upscaled equations. In particular, these numerical experiments show how the internal distribution of the permeability and porosity affect the effective behavior of the flow.

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Multiscale computation of pore-scale geomechanics

Authors: Yashar Mehmani[1]; Nicola Castelletto[None]; Hamdi Tchelepi[None]

[1] *Stanford University*

Corresponding Authors: tchelepi@stanford.edu, castelletto1@llnl.gov, yashar.mehmani@gmail.com

Mechanical deformation of porous media is relevant to several subsurface applications such as the safe storage of CO2 in geological formations, geothermal energy extraction, and unconventional hydrocarbon production. The macroscopic solid mechanical behavior and properties of a porous medium (e.g., elastic moduli, Biot coefficients) emerge out of the specific microstructural arrangement of its constituent minerals/crystals and any possible contact defects between them. A better understanding of these microscopic interactions will lead to more accurate macroscopic models and constitutive relations that are useful in practice. Advances in microscopic image-based characterization, such as X-ray μCT and EDS, have enabled the mapping of the complex geometry and chemical composition of a porous specimen. While such images can be used in subsequent microscale calculations to understand macroscale physics, current modeling capabilities are either too approximate or overly expensive. This work aims to strike a balance by reformulating the governing equations and the computational machinery needed to solve them. We specifically consider the case of a consolidated porous medium (a rock from the deep subsurface) exhibiting mineralogical heterogeneity and micro-cracks. A multiscale method is then developed that produces approximate but accurate predictions of the displacement and stress fields within the samples. Any remaining errors can be arbitrarily reduced through a built-in iterative scheme. An algebraic interpretation of the multiscale method as a linear preconditioner is also briefly discussed. The approach is amenable to computing on parallel machines.

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Robust and efficient solvers for flow in deformable porous media

Author: Florin Adrian Radu[1]

[1] *University of Bergen, Norway*

Corresponding Author: florin.radu@uib.no

In this talk we will discuss first solvers for the linear, quasi-static Biot equations [1, 2]. Monolithic and splitting schemes will be presented. Further, efficient numerical schemes for nonlinear versions of Biot´s model will be considered. This includes nonlinear Lame parameters or compressibility 3, large deformations [4] or unsaturated flow and deformation 5. The linearization is performed by using either the Newton method or the L-scheme [6, 7]. Illustrative numerical examples will be shown.

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Multiple-method pore structure characterization of Upper Cretaceous lacustrine shale from Songliao Basin in Northeast China

Author: Mianmo Meng[1]

Co-authors: Hongkui Ge [2]; Yinghao Shen [2]; Qinhong Hu [3]

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

[2] *China University of Petroleum, Beijing*

[3] *The University of Texas at Arlington*

Corresponding Author: mengmianmo@outlook.com

Lacustrine shale in China holds a vast resources of oil, and the understanding of its pore structure is significant for cost-effective development of this unconventional resource. The pore structure of lacustrine shale in Qingshankou formation from Songliao Basin were investigated with multiple and complementary methods, including scanning electron microscope (SEM), mercury intrusion porosimetry (MIP), low temperature nitrogen adsorption (NA), low field nuclear magnetic resonance (NMR), and computed tomography (CT). The studied lacustrine shale at a maturity of 0.5~1.09, the width of its inorganic pore can be up to 2.74 μm; one organic pore was observed to be 2.21 μm, and there is a crack at 399 nm in width probably caused by organic matter shrinkage. Comparing the pore size distribution between NA and MIP methods, the pore volume controlled by throat can be 18 times of the corresponding throat volume. From NMR results, about 90% pores are distributed from 0.01 ms to 1 ms in the relaxation time and the summit of left peak is near 0.1 ms, and microcracks mainly range from 2 ms to 10 ms, which may be correspondent to the pore size from 2 μm to 8 μm reflected by CT results. The fractal characteristic was investigated with NA data using the fractal Frenkel-Halsey-Hill (FHH) method. The fractal dimension D1 can reflect the roughness of pore surface; the higher the D1 is, the rougher the pore surface is. The dimension D2 can reflect the pore structure complexity, with a higher D2 value reflecting a more complex pore structure. The fractal dimension D1 ranges from 2.1471 to 2.4765, and the fractal D2 distributes from 2.4245 to 2.8297 in lacustrine shale, which indicated that lacustrine shale has a smooth pore surface and a complex pore structure. Overall, this research benefit to understand the pore structure of lacustrine shale.

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Reconstruction of Porous Media Based On Variational Autoencoders Method Using 2D Slice

Author: Yurun Li[1]

Co-authors: Qihong Feng [1]; sen wang [1]; jiawei ren [1]

[1] *china university of petroleum east china*

Corresponding Authors: 1404020204@s.upc.edu.cn, 17854227493@163.com, 942317501@qq.com, 645934634@qq.com

The reconstruction of the three-dimensional digital cores based on fewer slices plays an increasingly important role in oil and gas research. The variational autoencoder contributes to the results by learning a stationary model that is optimized with the cost of cross-entropy from the normal distribution. In the paper, we show an accuracy and robustness variational autoencoder of digital reconstruction improved by utilizing a generalization of cross-entropy and divergence. 3D digital core reconstruction based on Variational Autoencoders, an unsupervised learning method through training encoder and decoder neural networks. The encoder consists of convolution layers, extracting the features from the input, and decoder is made of deconvolution layers correspondingly, multiplying each receptive field by a filter elementwise. Between the encoder and decoder, the parameters of a Gaussian distribution from training data. The parameters of Gaussian distribution, the information for recurrence, represent the latent space of the digital rock. The decoder reconstructs the information into a new figure from the parameters. We train the network through the training data and reconstruct digital rock through a high-dimensional trajectory. We use the Berea digital rock, the imaging from the Berea SandstoneTM Petroleum Cores(Ohio, USA), as train data to optimize the VAE model. The trajectory is defined as a multinomial, which is continuous in high-dimensional space to guarantee the results are continuous in high-dimension as well. The results show that the trajectory has a close relationship with the digital rock. A good trajectory reconstructed 3D digital core has better pore connectivity and is similar to the real pore space. All in all, the effect is dependent on parameters distribution of latent space and the trajectory selected. The VAE model shows good performance in reconstruction of digital rock with less information once a network is trained. The trajectory in latent space is the key to control the structure of digital rock.

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Micro-macro Models: The Next Generation Models for Reactive Flow and Transport Problems in Porous Media ?

Author: Peter Knabner[1]

[1] *University Erlangen-Nürnberg Department Mathematics*

Corresponding Author: knabner@am.uni-erlangen.de

In porous media and other complex media with different length scales, (periodic) homogenization has been successfully applied for several decades to arrive at macroscopic, upscaled models, which only keep the microscopic information by means of a decoupled computation of "effective" parameters on a reference cell. The derivation of Darcy's law for flow in porous media is a prominent example. Numerical methods for this kind of macroscopic models have been intensively discussed and in general, are considered to be favourable compared to a direct microscale computation. On the other hand, if the interplay of processes becomes too complex, e.g. the scale separation does not act in a proper way, the porous medium itself is evolving, ..., the upscaled models obtained may be micro-macro models in the sense, that the coupling of the macroscopic equations and the equations at the reference cell is both ways, i.e. at each macroscopic point a reference cell is attached and the solution in the reference cell depends on the macroscopic solution (at that point) and the macroscopic solution depends on the microscopic solutions in the reference cells. At first glance, such models seem to be numerically infeasible due to their enormous complexity (in d+d spatial variables). If on the other hand this barrier can be overcome, micro-macro models are no longer a burden but a chance by allowing more general interaction of processes (evolving porous media, multiphase flow, general chemical reactions, ...), where the microscopic processes \compute" the constitutive laws, which need longer be assumed (similar to the concept of heterogeneous homogenization). We will discuss various examples and in particular numerical approaches to keep the numerical complexity in the range of pure macroscopic models.

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Thin film flow: fluid transport via thin liquid films in slow porous media flows

Author: Marcel Moura[1]

Co-authors: Knut Jørgen Måløy [1]; Eirik Grude Flekkøy [1]; Gerhard Schäfer [2]; Renaud Toussaint [3]

[1] *PoreLab, Univerisity of Oslo, Norway*

[2] *LHyGeS, CNRS, University of Strasbourg, France*

[3] *IPGS, CNRS, Univ. Strasbourg, France & PoreLab, Univerisity of Oslo, Norway*

Corresponding Authors: renaud.toussaint@unistra.fr, schafer@unistra.fr, k.j.maloy@fys.uio.no, marcel.moura@fys.uio.no, flekkoy@fys.uio.no

The standard liquid transport processes in porous media happen through the usual network of interconnected pore bodies and pore throats (here called the *primary network*). When a non-wetting phase displaces a wetting phase from a porous sample (drainage), thin films of the wetting phase are bound to be left on the surface of the constituting grains (for example when air displaces water from a porous rock, thin films of water are left behind, covering the rock grains). Under certain conditions, isolated liquid films can eventually merge, forming a *secondary network* of interconnected films and capillary bridges that can effectively enhance the overall connectivity of the medium and act as a new pathway for fluid transport. We have performed experiments using transparent networks with the objective of studying these unconventional transport processes. Our setup allow us to directly visualize the secondary network in the sample. We show how fluid bodies that are not linked via the primary network can actually be connected via the secondary network. This connection has important consequences for processes such as the dispersion of pollutants in soils and the transport of nutrients to plants in arid regions.

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CO2-Regulated Octane Flow in Calcite Nanopores from Molecular Perspectives

Authors: WEI ZHANG[1]; Zhehui Jin[2]; Qihong Feng[3]

[1] *China University of Petroleum*

[2] *University of Alberta*

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

Corresponding Authors: fengqihong@gmail.com, weizhang0919@hotmail.com, zhehui2@ualberta.ca

Thanks to the enhanced oil recovery (EOR) and the potential of geological CO2 sequestration, CO2 injection into unconventional shale/tight reservoirs has gained extensive attention among scientists and engineers in recent years. Unlike conventional reservoirs, shale/tight reservoirs contain an enormous number of nano-sized pores. During EOR process in shale/tight reservoirs, understanding the effect of CO2 on oil flow in nanoporous media is imperative to the prediction of ultimate oil recovery and optimization of well productivity. In this work, we use molecular dynamics (MD) simulations to investigate the effect of CO2 on nC8 flow in calcite nanopores. Without CO2, nC8 forms layering structures on calcite pore surface, while its first adsorption layer is immobile under a pressure gradient. As CO2 content increases, CO2 molecules are preferably adsorbed on calcite pore surface forming a thin CO2 film, while nC8 molecules are gradually depleted from the surface. The thin CO2 film is immobile under a pressure gradient. When CO2 content is low, as it is predominantly adsorbed on the pore surfaces, it has a negligible effect on oil flow. As CO2 content further increases, only after the first nC8 adsorption layer is completely replaced by CO2, CO2 can mix with nC8 in the regions away from the pore surfaces to reduce oil viscosity. As a result, nC8 flow rate in calcite nanopores is dramatically enhanced. For a given calcite nanopore, there is a critical CO2 content

beyond which the oil viscosity can be reduced and oil flow is subsequently enhanced; below this content, while CO2 can displace the first oil adsorption layer on pore surface, it does not affect the pressure-driven oil flow. Our study explores the role of CO2 on oil flow in calcite nanopores and provides important insights into the prediction of oil flow rate and rational optimization of CO2 EOR process in shale/tight formations.

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A novel approach to identify hydraulic conductivity fields that best approximate geological uncertainties via unsupervised learning techniques and Wellhead Protection Area Analysis

Author: Abelardo Rodríguez-Pretelín[1]

Co-author: Wolfgang Nowak [2]

[1] *formerly at Institute for Modelling Hydraulic and Environmental Systems (IWS)*

[2] *Institute for Modelling Hydraulic and Environmental Systems (IWS)*

Corresponding Authors: wolfgang.nowak@iws.uni-stuttgart.de, abelardo.rodriguez.pretelin@gmail.com

Typically, in order to deal with geological uncertainty during WellHead Protection Area (WHPA) analysis, groundwater modelers use an ensemble of many hydraulic conductivity realizations or other multiple representation approaches to capture the influence of uncertain hydrogeological conditions, generally using Monte Carlo simulation 1. Each of these realizations depicts a different hydraulic conductivity field that leads to distinctive contour lines and streamlines 2 and thus to different capture outline solutions. The straightforward analysis of such methods is statistical aggregation over the ensemble of capture realizations which summarizes the results to the decision maker in order to provide a simple communication of uncertainties. The obtained output is a well capture probability map with values ranging from 0 to 1 that expresses the probability of well pollution in case of spill events for each location inside the probabilistic WHPA delineation 3, [4], 5.

The involved Monte Carlo simulations are already expensive as they trigger a loop over many model calls. However, more complex analysis may trigger even more loops nested inside or outside the Monte Carlo loop. Such more complex aspects might be, in the case of WHPA delineation, transient simulation of transport towards a well (time loop inside the Monte Carlo loop) or optimization of adaptive pumping rates (optimization loop around the Monte Carlo loop). In such cases, it is tempting to represent uncertainty using a limited set of hydraulic conductivity realizations.

One possible strategy to reduce this computational cost is to substitute the Monte Carlo loop with a limited set of aquifer realizations according to the modeller own experience and knowledge. However, this manual interpretation of geological uncertainty might bring on bias into the overall result. This could lead for instance in over-confident management strategies for groundwater protection that perform worse in practice than what is expected during the optimization and decision making. A less subjective methodology that has been used to identify such representative subsets of realizations is unsupervised learning, for example clustering. Cluster analysis searches, within a low-dimensional representation of the ensemble, for commonalities among realizations based on some distance measures. The number of clusters required to represent the total ensemble is an indicator for the structure of knowledge in the chaos of uncertainty, and a small set of models (one at the center of each cluster) is used as condensed, yet comprehensive, set of hypothesis to represent the relevant aspects of uncertainty.

In this project, we apply clustering techniques to speed up WHPA analysis in a transient-transport context, combined with optimal pumping management. To the best knowledge of the authors, there is only one study addressing clustering in groundwater flow modeling. Alzraiee and Garcia (2012) [6] compared the cumulative distribution function of hydraulic heads between an ensemble of 400 hydraulic conductivity fields and distinctive subsets using different clustering algorithms and distance criteria. We aim to deepen the use of clustering techniques in groundwater flow modeling, evaluating the effects in transport modelling, particularly addressing WHPA analysis.

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Production Enhanced Potential Evaluation and Integrated Design for Horizontal Wells Energized Fracturing — Case Study on Chang 7 Tight Reservoir, Ordos Basin

Author: Guanqun Li[None]

Co-authors: Yuliang Su [1]; Wendong Wang [2]; Xia Du

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

[2] *School of Petroleum Engineering, China University of Petroleum (East China), 266580, Qingdao, China*

Corresponding Authors: duxia_upc@163.com, guanqun_li@163.com

As the pressure of Chang 7 tight reservoir is too low to reach failure pressure, energized fracturing is required to supply formation energy by water injection before hydraulic fracturing. Although applied in several oilfields, detailed mechanisms associated with energized fracturing and fracture propagation modes are still poorly understood. In this work, we established a numerical simulation model, in which stress field and seepage field are coupled to simulate the increased energy through water injection, the propagation of hydraulic fractures after energized, formation pressure maintenance time and production enhancement.
A set of high-resolution 3D reservoir models are constructed based on the field data obtained from the tight reservoir in Changqing Oilfield. A 4D ground stress field model for energized fracturing is subsequently constructed to simulate the in-situ ground stress field, stress field after water injection, and energized fracturing stress field. Discrete fracture network (DFN) models, which take stress

field and seepage field coupling into account, are examined to simulate the propagation of the fracture in the tight reservoir after energized. After that, the critical parameters of energized hydraulic fracturing are optimized to maximize single-well production.
After injection, the formation pressure rises to reduce the effective stress, so that the Mohr's Circle shift to the left, and the probability of shear slip is increased, which improves the success of fracturing. It is further observed that the injection flow rate is positively related to stimulated reservoir volume(SRV) and the production; however, more water injection, slower production decline rate. When the injection flow rate is more than 20,000m3, the increase of formation pressure is not apparent. The daily oil production of the energized fracturing is 2-3 times larger than the traditional hydraulic fracturing. Therefore, the energy of formation, the volume of the remote fractures, and the fractures capacity are enhanced by energized fracturing.
This work presents a set of detailed simulation studies to examine the distribution of ground stress and the propagation of fractures in hydraulic fracturing after water injection. A novel, yet practical, model is implemented to effectively simulate the coupling of stress and seepage fields, as well as to realize the pattern of fractures propagation in energized fracturing. The modeling method can optimize the injection flow rate and determine the optimal critical parameters for the injection of enhanced oil production. The results have revealed that water injection before fracturing can change the formation stress field, along with the associated implications on fractures propagation and production enhancement.

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Opalinus Clay experimental dataset with High Pressure Sorption, review and application to Pore Network Modelling

Authors: Georgy Borisochev[1]; Andreas Busch[1]; Jingsheng Ma[1]; Lin Ma[2]

[1] *Heriot-Watt University*

[2] *University of Manchester*

Corresponding Authors: gb168@hw.ac.uk, jingsheng.ma@hw.ac.uk, a.busch@hw.ac.uk, lin.ma@manchester.ac.uk

Mudrocks contribute around 70% of all sedimentary rocks in the earth crust. Recent technological advances make mudrocks an important target for oil and gas exploration; at the same time, they serve as seals for carbon storage reservoirs or radioactive waste repositories. Development of such projects requires fluid flow prediction, using reservoir modelling on the formation scale. Yet, necessary upscaling of rock properties such as absolute and relative permeabilities and capillary pressures cannot be obtained easily through conventional core analysis due to the highly multiscale nature of mudrocks. This issue creates the need for predictive modelling at pore scale, and with pore sizes varying from nanometers to micrometers. As such, a complete characterisation of pore space is necessary across all scales in order to create a comprehensive flow model.
Opalinus Clay, obtained from the Mont Terri underground rock laboratory in Switzerland has been thoroughly researched in recent years. A complete dataset of mineralogical and petrophysical properties has been summarised, providing input to such flow models. Specific experimental data includes focused ion beam scanning electron microscopy (FIB-SEM), small angle neutron and X-Ray scattering, low pressure N2 sorption, mercury injection porosimetry and a variety of complementary methods.
In addition to available datasets, high pressure sorption experiments were carried out using a manometric setup, allowing to evaluate the amount of physiosorbed gas in the pore space at different pressures and temperatures, resembling subsurface conditions. Four isotherms were measured at 45oC and pressures up to 20 MPa using methane as a sorbate. A dry sample was analysed to calculate the maximum excess sorption value of 0.55 mmol/g. Three samples were saturated with water

at 22, 24 and 40 % relative humidity. A general trend or reduction of adsorption capacity with increasing water saturation was observed.
Pore Network Modelling (PNM) is a method of pore space simulation, which approximates pore bodies and throats as nodes and bonds and models flow semi-analytically. Such approximation makes PNM significantly more computationally efficient than direct numerical methods. Pore network models were generated at different scales using FIB-SEM images and stochastically using a variety of pore size distributions collected for Opalinus Clay. These networks have been combined and simulated using a Slip- and Knudsen-flow solver to improve prediction of upscaling parameters, such as absolute and relative permeabilities and capillary pressures. Methane adsorption isotherms have been used to predict the amount of gas adsorbed within the model to adjust effective pore and throat widths that are open to flow.

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Generation of a micro-earthquake clouds induced by the arrival of nonlinear fronts of pressure and temperature

Authors: Arrigo Caserta[1]; Roman Kanivetsky[2]; Ettore Salusti[3]

[1] *INGV*

[2] *University of Minnesota*

[3] *CNR*

Corresponding Authors: ettore.salusti@gmail.com, arrigo.caserta@ingv.it, kaniv001@umn.edu

Deep geothermal or hydrocarbon reservoirs are often analyzed by observing the evolution of micro-earthquake clouds, generated by a deep fluid injection, which can cause deep fronts of fluid pressure P and rock-fluid temperature T. Here we focus on the evolution of micro-earthquakes generated by an "impulse" of pressurized cold fluid in a deep brittle media, or by a time dependent pressure forcing. Such impulse, or forcing, originates local gradients of pore pressure, which in turn generate fluid movements with some amounts of kinetic and/or thermal energy.
We therefore discuss a two-equations nonlinear model for pore pressure and fluid/rock temperature dynamics in porous rocks. Of particular interest is that, by coupling these two equations, we obtain a Burgers-like nonlinear equation, which represents one of the most studied, nonlinear mathematical equation in physics. Solution of our analytic model show both solutions as mild transients due to the classical linear diffusion and nonlinear "solitons", namely sharp and quick nonlinear transients of temperature and pressure. The latter case, indeed, occurs where the injection pressure is larger than (or comparable with) the minimum principal stress Σ.
In addition, since the idea of a constant rock permeability is in contrast with many field observations, we investigate the effect of a pressure-dependent permeability. We therefore focus on the effect of a small zone of inhomogeneous anisotropic rock parameters on a local formation of a micro-earthquake, and its time-space evolution.
This allows to discuss our main question, i.e. to infer the fluid dynamics and the geological local characteristics that are necessary to trigger a micro-earthquake event, in the diffusive or in a soliton cases. We thus consider fairly realistic condition, although maintaining an analytic, diagnostic approach. Finally, we apply all this to different rocks, such as sandstones, granites, marble, etc.

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Capillary heterogeneity trapping within the Captain Sandstone - a core to field scale study

Author: Catrin Harris[1]

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

[1] *Imperial College London*

[2] *CSIRO Energy*

Corresponding Authors: a.muggeridge@imperial.ac.uk, s.krevor@imperial.ac.uk, adwjones1@gmail.com, ch2919@ic.ac.uk, samuel.jackson@csiro.au

The aim of this paper is to understand the effect of natural rock heterogeneities on capillary trapping, over different length scales. Capillary pressure barriers trap CO2 at saturations greater than expected from residual trapping processes alone 1. Capillary trapping is a key mechanism underpinning storage security, potentially immobilising a significant proportion of the CO2 plume. Recent advances in core analysis show both fluid migration and capillary trapping are sensitive to spatial heterogeneity [1,2]. Current models describing capillary heterogeneity trapping, resulting from CO2 plume interactions with rock heterogeneities, are limited 3.

In this paper we apply a multiscale approach, combining petrophysical characterisation and numerical modelling, to create a physics-based representation of capillary heterogeneity trapping at the field scale. Previous research has focused on the impact of capillary heterogeneity in developing local saturations during drainage [4]. This project will extend to imbibition processes, observed experimentally to depend on heterogeneities 5. Models will account for relative permeability and capillary pressure hysteresis, often omitted from idealised models [6]. Two-region models have been created using a commercial reservoir simulator to study the physical basis of capillary heterogeneity trapping. The parameters influencing the length scale of capillary heterogeneity trapping are explored to define an improved dimensionless capillary number [7]. Additionally, the parameter space in which capillary heterogeneity trapping dominates pore scale trapping is studied. The resulting dimensionless capillary number improves understanding of the controls on capillary heterogeneity trapping. The results are compared with an analytical model by Dale and Ekran (1994), extended to account for imbibition processes [8].

The insights from the two-region models are applied to the Captain Sandstone, to study the effect of natural rock heterogeneities on capillary trapping within a target storage site [9]. The Captain Sandstone represents an archetypal CO2 storage unit, a sandstone aquifer, demonstrative of a poorly consolidated North Sea formation [4]. A comprehensive database has been produced through characterisation of 48 core plugs over a 65m interval of the Captain D Sandstone, Goldeneye formation, UK North Sea. Steady-state core flooding experiments using medical x-ray CT provide a detailed characterisation of continuum multiphase flow properties, including residual trapping characteristics, over cm scales. The data will be used to create 1D fine models of the Captain sandstone to evaluate capillary heterogeneity trapping during imbibition.

Our results demonstrate that heterogeneity results in a higher initial saturation from which imbibition occurs hence the residual saturation is naturally higher relative to the homogenous case. In addition, the residual saturation is higher than predicted by a typical residual trapping model because capillary pressure barriers trap CO2 at saturations greater than expected from residual trapping processes alone.

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Quality assessment and parameter estimation of post-laminar flow models

Authors: Mohaddeseh Mousavi Nezhad[None]; Alberto Guadagnini[1]

[1] *Politecnico di Milano*

Corresponding Authors: m.mousavi-nezhad@warwick.ac.uk, alberto.guadagnini@polimi.it

Post-laminar flows take place at high seepage velocities through a variety of engineered and natural porous media, such as gas turbine blades, catalytic converters in automobiles engines, fractured rocks, near-wellbore regions in subsurface reservoirs, and river sediments. Inertial forces are documented to markedly contribute to give rise to complex flow patterns as fluid velocity increases. These, in turn, impact chemical transport processes [e.g., 1 and 2]. Several studies aim to enhance our understanding about these flow and transport processes upon relying on direct observations through experiments performed at various scales. Empirical formulations have been presented to embed high velocity inertial effects in modeling the relationship between fluid velocity and pressure drop. Most of the available models include different parameters, whose estimation under diverse flow regimes is a key challenge 2. Currently used techniques for parameter estimation in the context of non-Darcy flow models are limited to simplified regression approaches based on experimental data. While it is generally recognized that model parameters depend on the morphology of the porous domain and flow characteristics, no unique values are proposed in the literature. This in turns reflects on the potential of a given calibrated model to be representative of diverse flow regimes.
Here, we rely on model identification criteria within the context of an inverse modeling approach based on a Maximum Likelihood framework to rank post-laminar flow models and investigate their skill in describing flow behavior under various flow regimes. Correlations between parameter estimates are investigated. Experimental data describing flow at diverse values of Reynolds number in randomly structured porous media are used to inform the inverse modeling approach. As such, the latter is formulated by including a regularization term to the objective function. This ensures porous media characteristics (e.g., intrinsic permeability) to be preserved while modeling the process over a

wide range of flow regimes. It is found that the Forchheimer parameters are directly correlated with the level of the heterogeneity of the porous media, and post-laminar flow is initiated by decreasing values of the Reynold's number as heterogeneity increases.

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Influence of the porous network on the conductive-radiative behavior of SiC-based cellular ceramics up to very high temperature

Authors: Benoit Rousseau[1]; Jerome Vicente[2]; Afeef Badri[None]; Yann Favennec[None]

[1] *CNRS LTeN UMR6607*

[2] *CNRS IUSTI*

Corresponding Author: benoit.rousseau@univ-nantes.fr

Refractory cellular materials 1 constitute an attractive class of porous materials for designing high-temperature energy conversion and transport systems and processes. Typical examples are volumetric solar receivers, gas burners, heat exchangers, thermal insulation walls. Their thermal behaviour at high temperature (T>1000 K) is poorly known today whereas the information is crucial for the global conception of industrial systems and processes 2. Several reasons can be proposed to explain such a situation going from the lack of experimental thermal data up to the complex texture which hampers the establishment of robust predictive law. To tackle this issue, one proposes in this presentation a numerical route which combines the numerical generation of cellular ceramics 3 thanks to an homemade software, genMat (C++, Qt) and a massively parallel finite element code developed in the FreFEM framework [4] which allows to treat simultaneously conductive and radiative heat transport at the pore scale. Three SiC-based cellular structures where the textural features are tuned will be confronted for same porosity and mean cell size: cubic-cell structures, Kevin-cell structures and random open-cell foams. The numerical samples will be fictitiously inserted between two opposite walls respectively maintained at 1200 K at one side and 1800 K at the other side, and under vacuum. The 3D temperature field in the porous volume will be given and the influence of the conductive radiative coupling will be discussed according to the Stark number which is commonly used in the radiative heat transfer community 5. This number allow to differentiate heat transport regime dominated either by conduction or by radiation. A practical guideline will be propose to tune the effective thermal conductivity at high temperature according to the pore network features.

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Impact of image resolution on quantification of mineral properties and simulated mineral reactions and reaction rates

Authors: Fanqi Qin[None]; Lauren Beckingham[1]

[1] *Auburn University*

Corresponding Authors: leb0071@auburn.edu, fzq0004@auburn.edu

Geological formations have great potential for CO2 sequestration, where ultimately CO2 is mineralized through geochemical reactions. Such reactions are expected to result changes in porous media including porosity and permeability. Reactive transport modeling can be utilized to simulate these complex reactions under reservoir conditions at different timescales. However, the variations in the estimated mineral reactive surface area can span 1 to 5 orders of magnitude, which could lead to large discrepancies in simulated results. Imaging has emerged as a powerful means of quantifying mineral properties including porosity, abundance, accessibility and accessible surface area which can be used to inform reactive transport modeling. It has been proven in previous work that accessible surface area better reproduced the observed dissolution rates in core-flood experiments and is quantifiable from images. However, the impact of image resolution on these estimated mineral properties is unknown. In this work, the impact of image resolution on estimated mineral properties is evaluated. Rock samples extracted from the Paluxy formation at Kemper County, Mississippi were imaged using scanning electron microscopy. Backscattered electron (BSE) and energy dispersive x-ray spectroscopy (EDS) images were captured under varying resolution from 0.34 to 5.71 μm. Imaging segmentation and registration were performed in Matlab and ImageJ. Mineral abundances and porosity quantified by pixel counting agreed relatively well with changing resolution. Mineral accessibilities measured from processed 2D SEM images were combined with 3D X-ray CT images to calculate mineral accessible surface areas. The accessibility of mineral phases with small-scale features decreases with decreasing resolution while variations in estimated accessible surface area are less than 1 order of magnitude. Image obtained data were used in CrunchFlow to simulate the CO2-induced reactions. Observed variations in accessible surface areas had small impacts on the simulated reactions. Additional simulations were carried out using BET surface areas from the literature and geometric surface areas, both of which are higher than image obtained surface areas. Large discrepancies were observed as different surface area values were used and each mineral phase was impacted by surface area variations to a different extent. Reactive phases (e.g. carbonates) were mostly impacted by surface area variations at short times (< 100s of hours) while the more stable phases (e.g. feldspars and clays) were impacted at longer times (> 100s of hours). Results can be used to inform the necessity of image processing to quantify accessible mineral surface area as it requires time and has high computational costs.

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valuation criteria of shale gas reservoir classification– taking Longmaxi formation in Pengshui area as an example

Authors: Ning Qi[1]; Mingyue Lu[2]

[1] *17806278642*

[2] *13136828339*

Corresponding Authors: 49142456@qq.com, 1430067486@qq.com

This paper takes the shale of the Lower Silurian Longmaxi formation in Pengshui area as the research object. the evaluation criteria of shale gas reservoir classification are determined by means of main / trace elements, high resolution field emission scanning electron microscope, focused ion beam scanning electron microscope, low temperature nitrogen adsorption, high pressure mercury injection, high pressure methane isothermal adsorption and field desorption. In order to reveal the enrichment law of atmospheric shale gas, the shale reservoir space of Longmaxi formation mainly includes intergranular pores, intragranular pores, organic pores and microfractures. Organic pore is the most important type of reservoir space, which is mainly oval, round or irregular, and the pore diameter is less than 110nm. Based on the fractal curve characteristics of nitrogen adsorption and high pressure mercury injection, the shale gas reservoir space is divided into macropores (> 110nm), mesoporous pores (25-110nm), small pores (5-25nm) and micropores (< 5nm). Micropores and micropores are mainly developed in shale reservoirs, but macropores and mesopores are not developed. The specific surface area of shale, the volume of micropores and micropores and the total pore volume show a decreasing trend from bottom to top, while the average pore diameter shows an increasing trend. According to the influence characteristics of micropores and micropores on the total desorption capacity in the field, the shale gas reservoir is divided into type I, II, III and non-reservoir. Based on the correlation between the total desorption capacity and TOC, the TOC classification limits of atmospheric reservoir are 4.3wt.%, 3.2wt.% and 0.3wt.%, while the TOC classification limits of overpressure reservoir are 4.5wt.%, 3.7wt.% and 0.5wt.%. The prediction model of specific surface area and pore volume of shale gas reservoir is established. the calculation results show that the pore volume and specific surface area of unit mass organic matter, clay minerals and brittle minerals are 0.213cm3/g and 360.01m2/g, 0.00513cm3/g and 10.96m2/g, 0.00351cm3/g and 1.62m ~ 2g, respectively, indicating that the degree of pore development in organic matter is much higher than that of clay minerals and brittle minerals.

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In Operando synchrotron microfluidics experiment and reactive transport modeling of acid erosion of carbonate fractures

Authors: Hang Deng[1]; Jeff Fitts[2]; Ryan Tappero[3]; Julie Kim[4]; Catherine Peters[None]; Qian Zhang[1]

[1] *Lawrence Berkeley National Laboratory*

[2] *Columbia University*

[3] *Brookhaven National Laboratory*

[4] *Princeton University*

Corresponding Authors: juliejk@princeton.edu, rtappero@bnl.gov, jpf2163@columbia.edu, cap@princeton.edu, hangdeng@lbl.gov, qianzhang@lbl.gov

In this study, we developed a custom microfluidic cell for an in operando synchrotron experiment using a suite of x-ray spectroscopic techniques. The experiment involves reacting a mineralogically heterogeneous rock from the Eagle Ford Shale with a channel flow of an acidic fluid. After 48 hours, we observed preferential dissolution of calcite from the rock surface, forming a porous altered layer with a sharp reaction front that varies spatially. The thickness of the altered layer varies between 200 to 500 um. The dissolution rate of calcite quantified from the x-ray attenuation data was 3e-4 mol/m2s, and decreased to 3e-5 mol/m2s after 24 hours as a result of the diffusion limitation through the altered layer. The surface area in the altered layer was found to be two orders of magnitude higher than in the intact matrix based on xCT analyses. As a result, Fe- and As- bearing mineral phases remaining in the altered layer become more accessible and the potential for mobilization of toxic metals such as Arsenic (As) will be increased. In our sample, quantification using XRF and XANES microspectroscopy indicated up to 0.5 wt% of As(-I) and 1.2 wt% of As(V) associated with ferrihydrite. Reactive transport modeling has also been used to simulate the development of the altered layer and to examine the impacts of initial structural and mineralogical heterogeneity on the spatial variation of the altered layer, which will provide important information for evaluating the mechanical strength of the altered fracture surface.

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Numerical Analysis of a Model of Biofilm Growth at the Pore-Scale

Authors: Azhar Alhammali[1]; Malgorzata Peszynska[2]

[1] *Imam Abdulrahman Bin Faisal University*

[2] *Oregon State University*

Corresponding Authors: mpesz@math.oregonstate.edu, aalhammali@iau.edu.sa

We consider a coupled system of two nonlinear partial differential equations (PDEs) that models biofilm growth and nutrient consumption in porous media at the pore-scale. One of the PDEs is characterized as a parabolic variational inequality due to the constraint on the volume of biomass. We approximate the model using two methods: i) Galrkin finite element method and ii) mixed finite element method. We show the well-posedness of the problem; we derive rigorous error estimate that is verified by numerical experiments. Furthermore, we conduct simulations in 2D and 3D that give qualitative results of the ones obtained by experiments and imaging.

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Buoyant convection in porous media: Multiple layers separated by an inclined permeability jump*

Authors: K. S. Bharath[1]; Morris Flynn[1]

Co-author: Chunendra Sahu [2]

[1] *University of Alberta*

[2] *University of Cambridge*

Corresponding Authors: cks34@cam.ac.uk, kattemal@ualberta.ca, mrflynn@ualberta.ca

We investigate, theoretically and similitude experimentally, the flow of a dense, Boussinesq plume through a two-layer porous medium characterized by a high permeability layer above and a low permeability layer below. The boundary, or permeability jump, between the upper and lower layers is inclined to the horizontal. On encountering the permeability jump, discharged plume fluid propagates up- and downdip as an asymmetric pair of (primary) gravity currents that, in turn, drain into the lower layer. When the upper and lower layers are assumed very thick, one can develop and numerically solve a coupled pair of non-linear advection equations with appropriate boundary conditions, this to predict the balance between advection and draining that may arise along a permeability jump. The model in question assumes Darcy flow and the existence of a sharp interface between the gravity currents and the surrounding ambient fluid. Similitude experiments highlight some of the limitations of this approach, i.e. they reveal the formation of two distinct density interfaces, which we label as either the bulk- or dispersed-interface. Notwithstanding this key difference between theory and experiment, both allow for a characterization of the transient- and steady-state behavior. Steady-state is defined as the point where, for both the up- and downdip gravity current flows, the inflow from the plume is precisely matched by the outflow due to draining. When these two flows balance, the gravity currents are said to have reached their run-out lengths. With reference to these run-out lengths, we conclude that the predictions associated with our sharp-interface model consistently fall between the bulk and dispersed interfaces measured from laboratory experiments.

Experimental attention is also focused on the case where the lower layer thickness is finite. Laboratory images reveal the formation of a pair of secondary gravity currents that form when the draining flow hits the bottom (impermeable) boundary. Depending on the layer thickness, the formation of secondary gravity currents exerts a significant influence on the dynamics of the primary gravity currents e.g. an arrested primary gravity current can be remobilized and so continue to flow up- or downdip along the permeability jump.

Through this work we attempt to address some of the key uncertainties in the field of groundwater contamination and acid-gas injection. These uncertainties include (i) the degree of asymmetry in the flow structure of the gravity as it propagates along an inclined and permeable boundary, (ii) the factors influencing the short- and long-term flow dynamics, and, (iii) the significance of dispersion and its relation to the angle of inclination of the flow.

*Funding Acknowledgment: NSERC

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Comparing chronopotentiometric behavior in homogeneous cation- and anion- exchange membranes

Authors: Chunyu Tian[1]; Kim Roger Kristiansen[2]; Signe Kjelstrup[3]; V. María Barragán García[4]

[1] *Deparment of Structure of Matter, Phermal Physics and Electronics, Faculty of Physics, University Complutense of Madrid*

[2] *PoreLab, Department of Chemistry, Norwegian University of Science and Technology, NTNU*

[3] *Norwegian University of Science and Technology, NTNU, Trondheim*

[4] *Department of Structure of Matter, Thermal Physics and Electronics, Faculty of Physics, Complutense University of Madrid*

Corresponding Authors: chunyita0329@sina.com, vmabarra@ucm.es, signe.kjelstrup@ntnu.no, kim.kristiansen@ntnu.no

Chronopotentiometry and current-voltage curves are useful for electrochemical characterization of ion-exchange membranes and for understanding rate limiting mass transfer processes in membrane systems. They permit investigation of transport phenomena in membranes and give information about relevant aspects of many electro-membrane applications. Ion transport plays a key part in electrodialysis, dialisys, electrochemical energy conversion, among others. A chronopotentiometry study was carried out with two homogeneous ion-exchange membranes, one cationic and one anionic. Different NaCl aqueous solutions with concentration in the interval 0.001 to 0.1 M were used as electrolyte. From the chronopotentiometric curves, the corresponding transition times were obtained. Current-voltage curves were also measured at the same concentrations in order to experimentally determine the values of the corresponding limiting current. It was found that, for some of the studied systems, two transition times occurred on the chronopotentiometric curve. One of them was very close to the theoretical transition time predicted by the Sand equation for a selective homogeneous membrane, mainly for the anionic membrane. The possibility of obtaining from this value information about ion transport numbers of the membranes was analyzed. A higher second transition time was also observed for anionic membranes with solutions of concentration up to 0.01M. For the cationic membrane, the second transition time was only observed at the lowest electrolyte concentration. In the rate-limiting current regime, current-induced phenomena appeared that did not occur at low current densities and the application of such currents could be considered as an emerging mode of process intensification. Water splitting is one of the main phenomena that may affect ion transfer, mainly through anion-exchange membranes, at high current regimes. The overpotential was estimated for each membrane system, observing that the second transition time was only presented at electric currents for which the overpotential exceeded the value of 1.2 V, suggesting that water electrolysis is the rate-limiting process.

Financial support from Banco de Santander and Universidad Complutense de Madrid under Project PR75/18-21589 is gratefully acknowledged. K.R.K. and S.K. is grateful to Research Council of Norway for project no 262644 PoreLab.

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Time-lapse imaging of fines migration within subsurface reservoirs

Author: Chenzi Shi[1]

Co-authors: Kevin G. Taylor [2]; Lin Ma [3]

[1] *Department of Earth and Environmental Sciences, University of Manchester*

[2] *Department of Earth and Environmental Sciences, University of Manchester*

[3] *Department of Chemical Engineering and Analytical Sciences, The University of Manchester*

Corresponding Authors: lin.ma@manchester.ac.uk, chenzi.shi@manchester.ac.uk, kevin.taylor@manchester.ac.uk

Fines migration may lead to formation damage through reducing permeability of subsurface oil, gas or water reservoirs and blocking pores under certain circumstances. This paper focuses on direct imaging and characterisation of fines migrations and deposition in reservoir-analogue glass beads

under laboratory experimental conditions using a combination of two-dimension (2D) in-situ time-lapse radiography and three-dimension (3D) X-ray tomography imaging techniques.

The experiment was conducted in a high-pressure flow cell set within a high flux X-ray tomography bay using an analogue model system which contains compacted glass beads (150μm–212μm) to provide a porous bed within the cell. A fluid (water) containing suspended calcium carbonate particles (≤50μm) was passed through the flow cell and glass beads. Fine particles deposited both inside the porous structure and upon the surface of the glass beads. X-ray tomography was used for pre- and post- scans to observe the volume and positions of the deposited fine particles as well as to determine the changes in the pore system of the porous sample. Time-lapse radiography was used to quantify the changes in internal structure during the experiment through time… At the beginning of the experiment, particles deposited upon the surface and the internal porous structure of the glass beads. The pressure increased gradually from 100psi to 700psi. From 107 seconds the deposited particles compacted on the surface forming a filter cake and internal pore volume decreased dramatically. From 315 seconds fine particles had filled all the inside part of the glass beads and increased further on the surface of the glass beads. The experiment lasted for 580 seconds in total.

The combination of 2D time-lapse radiography with 3D X-ray tomography is a powerful way to image and characterise fines migration within reservoir analogues. The spatially and temporally quantified results have significantly improved the understanding of the flow behaviours of suspensions, the internal structure variation, and the processing of the analogue model in the subsurface systems. This study has wide applications in subsurface reservoirs, such as hydrocarbon extraction, geothermal utilisation, carbon storage, and gas storage (e.g. compressed air, natural gas and hydrogen) to enhanced geo-energy recovery and subsurface energy efficiency.

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Swelling properties in reinforced polymeric ion-exchange membranes

Authors: Íñigo Lara[1]; Sagrario Muñoz[1]; V. María Barragán García[2]

[1] *Department of Structure of Matter, Thermal Physics and Electronics, Faculty of Physics, Complutense University of Madrid*

[2] *Department of Structure of Matter, Thermal Physics and Electronics, Faculty of Physics, Complutense University of Madrid*

Corresponding Authors: vmabarra@ucm.es, smsm@ucm.es, inigolar@ucm.es

Swelling properties are fundamental on the behavior of ion-exchange membranes in many applications. Water content of the membrane affects the performance of applications such as fuel cells due to the membrane electric conductivity strongly depends on the hydration membrane conditions. Moreover, water sorption into the membrane could be accompanied by changes in its dimensions and thus affect the membrane stability. Develop membranes with both low swelling and high water uptake is thus an important issue.
In this work, water uptake and dimensional changes after immersion in liquid water were measured for the non-reiforced Nafion 117 membrane and for different reinforced polymeric ion-exchange membranes in order to analyze the influence of the reinforcement on the membrane structure in its swelling properties. Reinforced Nafion N324, and Fumasep FKS-PET-75 and FAS-PET-75 membranes were studied. Changes in mass, thickness and area of the membrane samples were measured as a function of time to analyze the kinetic of the water adsorption process and to estimate the equilibrium values. Lower values for water uptake and wet porosity were observed for reinforced

membranes. The thickness change was similar for all membranes, but reinforced membranes exhibited improved area stability compared with the non-reinforced Nafion membrane.

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Spectral time-dependent solutions for natural convection in porous enclosure

Authors: AMIN FAHS[1]; ALI ZAKERI[2]; ADRIEN WANKO[3]

[1] *Laboratory ICube, University of Strasbourg*

[2] *K.N.Toosi University of Technology, Faculty of Mathematics*

[3] *Laboratoire ICube De mathématique, Des sciences l'ingénieur, de L'informatique et de l'imagerie*

Corresponding Authors: wanko@unistra.fr, fahs.amin@etu.unistra.fr, azakeri@kntu.ac.ir

In this work, we have investigated time-dependent natural convection in a square porous cavity. A high accurate reference solution is developed using the Fourier-Galerkin (FG) spectral method applied to the stream function formulation of the governing equations. In the spectral space, this method leads to a system of nonlinear differential-algebraic equations that we simplify in ordinary differential equations and integrate in time using the variable order Runge-Kutta method. Two configurations dealing with transient and unsteady regimes are considered. For each configuration, the solution is derived for a wide range of Rayleigh numbers. The developed FG solution shows high accuracy with a reduced computational cost. It is in excellent agreement with a finite element solution. The FG solution is used to provide physical insight on the effect of time variation on the mechanisms of NC. The results provide a set of high-accurate data that can be used for benchmarking numerical codes of heat transfer in time-dependent configurations.

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Experimental Study on the Performance of a Hybrid Evaporator Wick with Bionic Topological Substrate

Author: Xin Cheng[1]

Co-authors: Jingyi Wu [2]; Guang Yang [2]

[1] *shanghai jiao tong university*

[2] *Institute of Refrigeration and Cryogenics, Shanghai Jiao Tong University*

Corresponding Authors: y_g@sjtu.edu.cn, jywu@sjtu.edu.cn, chengxin-17@sjtu.edu.cn

Development of more intelligent, integrated and powerful electronic systems requires effective thermal management technology to ensure reliable operating temperature. Based on the liquid-vapor phase-change theory, capillary evaporation heat transfer has been widely used in many fields, such as aerospace, energy, nuclear industry and electronics industries, by greatly increasing heat transfer area and spontaneously maintaining liquid supply. Over the years, many researchers have made excellent contributions to the enhancement of heat transfer by capillary wicks, which composed of microchannels, microcolumn arrays, sintered particles, sintered meshes or nanowire arrays. However, due to the intricate interplay between flow resistance and capillary force in porous structure, we cannot optimize the capillary wicks towards the integrated objective of maximum capillary pumping while increasing the evaporation thin film region of meniscus in a homogeneous wick. In this study, we designed a hybrid evaporator wick composed of a bionic topological substrate and an auxiliary liquid supply layer to meet the urgent heat dissipation requirements of high heat flux hotspots. The hybrid wick decouples the flow resistance and capillary driving force in the wick, which is effective for improving the performance of the evaporator wick. Therefore, in order to explore the advantages of the hybrid wick, an experimental investigation has been conducted.
Firstly, we fabricated a micropillar array structure with bionic vein channels on a silicon substrate by deep reactive ion etching technology, and then bonded a metal foam with vapor channels as the liquid supply layer on the micropillars. We studied the flow characteristics of the bionic topological substrate and compared it with the uniform micropillar array. The results show that the bionic topological structure significantly improves the fluid absorption rate of the capillary structure. Simultaneously, we studied the capillary characteristics (K/reff) of copper-based graphene foam and copper foam with the same geometric parameters through capillary rate-or-rise experiment, and found that the capillary performance of copper-based graphene foam is better than that of copper foam. However, due to the effect of contact thermal resistance, the nano-scale rough structure on the surface of the copper-based graphene foam framework failed to exhibit the expected effect of enhancing evaporation. Then, the heat transfer coefficient (HTC) and the critical heat flux (CHF) of the hybrid wick is investigated by a self-built experimental system for achieving saturated environment. The results show that the designed hybrid wick has a higher critical heat flux and higher heat transfer coefficient than traditional sintered wicks. Moreover, a comprehensive optimization of multi-parameters will be conducted, including the arrangement of vein channels, the geometric parameters of the micropillar array, the thickness of the liquid supply layer, etc.

Keywords Hybrid wick, Capillary evaporation, Bionic topology, Critical heat flux, Flow characteristics

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A generalized finite volume method for density driven flows in porous media

Author: Yueyuan Gao[1]

Co-authors: Danielle Hilhorst [2]; Huy Cuong Vu Do [3]

[1] *MAthAM-OIL, AIST*

[2] *CNRS and Université Paris-Saclay*

[3] *University of Science, VNU-HCMC*

Corresponding Authors: vdhuycuong@yahoo.com, yueyuan.gao@aist.go.jp, danielle.hilhorst@math.u-psud.fr

We consider a model describing the interaction between flow and transport in a porous medium coupling with heat transfer. The benchmark is proposed in the documentation of the computer program SEAWAT. It consists in a two-dimensional cross section of a confined coastal aquifer initially saturated with relatively cold seawater (concentration 35 kg/m3 and temperature 5 C). And warmer fresh water (concentration 0 kg/m3 and temperature 25 C) is injected into the aquifer along the left boundary. The fresh water and the sea water mix together and discharge into a vertical seaward boundary. This system models for example the extraction of salt water containing lithium from salt lakes.

Specifically, we solve a system for the hydraulic water head, the concentration and the temperature. We apply a semi-implicit scheme in time together with a generalized finite volume method SUSHI and adaptive meshes for the numerical solution.

It is joint work with Danielle Hilhorst and Huy Cuong Vu Do.

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1210

Pore-by-pore wettability characterization in sandstone and carbonate rocks

Author: Gaetano Garfi[1]

Co-authors: Maja Ruecker [1]; Qingyang Lin [1]; Steffen Berg [2]; Cédric M. John [1]; Sam Krevor

[1] *Imperial College London*

[2] *Shell Global Solutions International B.V.*

Corresponding Authors: s.krevor@imperial.ac.uk, q.lin11@imperial.ac.uk, m.rucker15@imperial.ac.uk, steffen.berg@shell.com, cedric.john@imperial.ac.uk, g.garfi17@imperial.ac.uk

Wettability is a key control of multiphase flow phenomena in porous rocks and substantially contributes to the efficiency of geological CO2 sequestration, hydrocarbon production and contaminant remediation. Due to the multi-scale heterogeneous nature of sedimentary deposits and the complexity of the interaction between crude oil and rock surfaces, characterizing the wettability of a reservoir is a challenging task. In Garfi et al. (2020) a theoretical and practical approach to rock wettability characterization based on the analysis of fractional fluid surface coverage of rock mineral surfaces was proposed and demonstrated. In this work, we build on and modify the approach to investigate fluid surface coverage on a pore-by-pore basis, therefore aiming at improving the spatial description of wettability.
By conducting the analysis of fluid surface coverage in X-ray micro-CT imaged rock samples during quasi-static fractional flow imbibition experiments, we characterize the wetting state of Bentheimer

sandstone and Estaillades limestone before and after wettability alteration. The oil phase drainage process was performed by centrifugation for both lithologies. Prior to imbibition, the samples were exposed to crude oil at 80℃ for 30 days in order to induce wettability alteration processes analogous to that observed in oil reservoirs.
We derive a model that allows for the quantitation of the wetting state of individual pores. We apply the model and find distinct wetting states for altered Bentheimer and Estaillades rocks; whereas Bentheimer is uniformly altered to an intermediate wet state, the pore structure of the Estaillades creates an approximately bimodal structure of oil wet and water wetting pores. Pore scale identification of the wetting state can be used directly in modelling, such as in the pore-by-pore assignment of a distribution of contact angles in pore network models.

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Continuous Surface Force Lattice Boltzmann Method for thin-gap flows - comparison with sharp interface FEM solutions.

Author: Michał Dzikowski[1]

Co-author: Marcin Dabrowski [2]

[1] *ICM, University of Warsaw*

[2] *Computational Geology Laboratory, Polish Geological Institute National Research Institute*

Corresponding Authors: mdabr@pgi.gov.pl, dziki01@gmail.com

Multiphase flows in narrow aperture domain with obstacles and roughness occur in both natural environments and technological devices. In low matrix permeability rocks such as shales, tight sandstones, and crystalline rocks, fluids move predominantly through networks of such rough-walled fractures. Typical examples of multiphase fracture flow in rocks include water and steam circulation in geothermal reservoirs, lateral and vertical spreading of dense non-aqueous phase liquids in shallow hydrogeological systems, particularly in partially saturated zones, and natural and stimulated hydrocarbon migration in petroleum systems.

In our work, we investigate various numerical approaches to immiscible two-component flow in the thin gap with obstacles in the presence of both surface tension and viscosity contrast. Presented studies are concentrated on low Reynolds number limit - namely the Stokes flow regime.
We compare the continuous surface flow approach with fully resolved sharp boundary with computational mesh conforming the fluids interface. The continuous approach was implemented using conservative phase-field solver for LBM proposed by [Geier, 2015] coupled with momentum equations using Continous Surface Force approach. It is worth noting, that most LBM multiphase methods are based on the pseudopotential approach and apply to miscible systems. Immiscible variants are also based on pseudopotential or directly on Cahn-Hilliard equation. In this worksurface tension force term is based on local curvature and phase-field gradient, the CSF model by Brackbill. To provide reference solution FEM Milamin solver is used, in which several methods were used for sharp interface representation. Presented LBM for immiscible flows was initially verified on versus known classical solutions. The amplitude of spurious currents, wetting angle recovery and convergence rate on simple tests were established. We choose simplified porous medium, an array of randomly placed

cylinders, to illustrate differences between methods. This simplified geometry is used to establish a stable range of Capillary number and viscosity ratio accessible to the proposed LBM method.

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Study on Mechanism of Nitrogen Stimulation Production Aided by Viscosity Reducer in common heavy oil

Authors: Yunong Zang[None]; Binfei Li[1]

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

Corresponding Authors: libinfei999@126.com, 43310095@qq.com

Nitrogen stimulation is a method of enhancing oil recovery in oilfields at present, because it utilizes the gravitational differentiation of nitrogen to excavate remaining oil. At the same time, nitrogen can supplement formation energy, increase elastic driving energy, increase oil well production in unit areas, and form foam oil. Improving the properties of the formation, such as the fluidity of crude oil, is of great significance for increasing oilfield production and efficiency. In this study, the nitrogen stimulation experiment and the viscosity reducer-assisted nitrogen stimulation experiment were conducted to analyze the different characteristics of the nitrogen oil and gas production and the effect of the viscosity reducer on the heavy oil production. At the same time, the microscopic visualization experiment was carried out to summarize and analyze the drop Viscosity aids heavy oil throughput mechanism. The results show that there are differences in the oil recovery rate of crude oils with different viscosities in the first two production cycles of nitrogen stimulation, and that in high-viscosity crude oils in the latter two cycles are higher than those in low-viscosity crude oils. Viscosity reducer-assisted nitrogen stimulation oil recovery in each cycle accelerates oil recovery rate and the duration of crude oil production is longer, and the viscosity reducer inhibits gas channeling during the production process to a certain extent, then it can improve crude oil recovery. The bubbles and emulsion formed by adding the viscosity reducer in the micro model reduce the gas phase mobility, increase the contact area and the degree of mixing between the viscosity reducer and the crude oil, thereby improving the crude oil recovery rate. In the field application, the measure of viscosity-reducing agent assists nitrogen suppresses the rise of water content in the oil layer and the water content of the formation decreases, which confirms the effect of this measure in controlling water and increasing oil and provides theoretical support.

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Mechanism study on water plugging and EOR by nitrogen foam injection in bottom-water reservoirs

Author: Danqi Chen[1]

Co-authors: Binfei Li [2]; Zhengxiao Xu [1]; Kun Liu [3]; Huiyu Yang [1]; Zheyang Liao [1]

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

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

[3] *Geological Research Institute of CNPC Great Wall Drilling Engineering Co., Ltd.*

Corresponding Authors: 1417668712@qq.com, 1445910379@qq.com, b18020040@s.upc.edu.cn, lkzzz.gwdc@cnpc.com.cn, libinfei999@126.com, cdq0813@163.com

Bottom-water coning occurs in middle and late stages of bottom-water reservoir development, resulting in various problems, such as rapid rise in water cut after water breakthrough, violent water flooding, low reservoir productivity, and lifespan shortage of development. Nitrogen foam has been characterized as having selective plugging capacity in layers with various permeability, low density, and oil-water sensitivity. Thus, water plugging with nitrogen foam is proved as an effective method for improving development during the high water-cut period of a bottom-water reservoir. This research first optimized surfactant solution system when subjected to high salinity and temperature by measuring the half-life period and foaming volume under various temperature and mineralization. Then, the paper investigated the nitrogen-foam flow behavior in porous media through single-tube sand-pack displacement tests and identified the effects of different factors on foam resistance such as injection function, gas-liquid volume ratio, injection rate, crude oil saturation and permeability. Two cores with different permeability were parallel-connected to simulate heterogeneous media and produced fluid from each core was separately collected to determine the shunt rate evolution during the displacement. The results indicate that gas-liquid mixed injection provides a greater pressure difference compared to slug injection and the optimal gas-liquid volume ratio is as 2:1. With the increase of foam injection rate, the displacement pressure difference first increases and then decreases when the flow rate reaches 2.52 m/d. The resistance factor and residual resistance factor increases as the increase of core permeability and foam presents a great plugging effect in areas with higher water-saturations. Based on dual-tube flow tests, foam injection can lead to a rapid shunt rate decrease for channels with high-permeability and it can realize the flow reversal in high and low permeability zones of porous media within the reservoir permeability contrast ratio of 6. This paper can provide references for the mechanism of nitrogen foam for water control and productivity increase.

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Shale gas productivity prediction and parameter optimization based on machine learning

Authors: Lu Qiao[1]; Shuangfang Lu[None]; Huijun Wang[None]; Zheng Fu[None]; Taohua He[None]

[1] *School of Geosciences, China University of Petroleum (East China)*

Corresponding Author: 18622375006@163.com

Abstract: Shale gas is the most potential energy in unconventional oil and gas resources. With the rapid development of drilling and fracturing technology, shale gas development has become a hot topic in the field of oil and gas development. However, the flow mechanism of shale gas reservoir is complex, and the impacts of geological and engineering parameters on the estimated ultimate

recovery of shale gas are not clearly understood. Therefore, it is significant to scientific and efficient development of shale gas reservoir to investigate the influence of geological and engineering parameters on shale gas production. In this paper, we performed history matching with X field gas production data. We employed the Design of Experiment to perform sensitivity studies with eight geological and engineering parameters such as porosity, formation permeability, pressure coefficient, gas saturation, number of fracturing stages, length of horizontal well, half fracture length, and fracture conductivity, and obtained the key parameters affecting gas production. Then, combining with the Gauss Process Regression (GPR) and Convolution Neural Network (CNN) method in machine learning field, taking the selected main control factors as the input parameters, we established the shale gas production model to predict the estimated ultimate recovery of shale gas under the influence of multiple non-linear factors. These two methods can not only provide high-precision solutions for high-dimensional and nonlinear problems, but also have better adaptability and generalization ability. The results demonstrated that the half fracture length, length of horizontal well, hydraulic fracture conductivity, hydraulic fracture spacing, porosity, and pressure coefficient had the most obvious influence on the production, and their optimized values were 300m, 3000m, 10mD·m and 20m, respectively. In addition, the gas production predicted by Gaussian process regression and convolution neural network is in good agreement with the actual value. This model is of great significance for the rapid establishment of output model and the formulation of optimal development plan.
Key words: shale gas ；productivity prediction ；parameter optimization ；machine learning

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Characterisation and 3D numerical modelling of multiphase flow in Carbonate rocks

Author: Nele Wenck[1]

Co-authors: Sam Krevor [1]; Samuel Jackson [2]; Ann Muggeridge [1]; Sojwal Manoorkar [1]; Alistair Jones [1]

[1] *Imperial College London*

[2] *CSIRO Energy*

Corresponding Authors: samuel.jackson@csiro.au, s.krevor@imperial.ac.uk, nele.wenck15@imperial.ac.uk, s.manoorkar@imperial.
a.muggeridge@imperial.ac.uk, adwjones1@gmail.com

Characterisation of multiphase flow properties, such as relative permeability and capillary pressure, is crucial in understanding and predicting large-scale fluid behaviour in the subsurface. Heterogeneity in the underlying rock structure, e.g. cross-bedding in clastic sands or vugs in carbonates, can cause large variations in porosity and permeability which manifest as capillary pressure heterogeneity [1,2,3,4,5]. At the low flow potentials encountered in the subsurface, these heterogeneities can significantly impact fluid flow behaviour, typically observed as large saturation variations within the rock [5,6,7]. With advances in non-invasive experimental techniques, which allow fluid displacements within a rock core to be imaged, a method to characterise capillary heterogeneity in sandstones was first developed by Krause et al. (2011), and later refined by Pini et al. (2012) and

Jackson et al. (2018). Driven by these successful results and recent findings on heterogeneity in carbonates [8], we extend and advance this workflow to model 3D capillary heterogeneity and multiphase flow in a wider range of rock cores, with a focus on Carbonate samples; Estaillades and Indiana limestone. The existence of micro-porous, vug and matrix regions within these samples significantly complicates the 3D characterisation, with heterogeneity impacts more prevalent than in sandstone systems. We present a generalised workflow, applicable to a wider range of rocks with multi-scale heterogeneity and facies. We validate this workflow with steady-state multiphase flow experiments at varying fractional flow and flow rate, at representative subsurface conditions. Overall, the modelling of the carbonate cores has shown that capillary heterogeneity generally raises the gas relative permeability at low capillary number, thus favouring gas flow.

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A quantitative method to compare Invasion Percolation models to high-resolution gas-injection experiments in sand

Author: Ishani Banerjee[1]

Co-authors: Anneli Guthke [2]; Cole Van de Ven [3]; Kevin. G. Mumford [3]; Wolfgang Nowak [4]

[1] *Institute for Modelling Hydraulic and Environmental Systems (IWS)/LS3, University of Stuttgart*

[2] *Institute for Modelling Hydraulic and Environmental Systems (IWS)/LS3, University of Stuttgart*

[3] *Department of Civil Engineering, Queens University, Kingston, Canada*

[4] *Institute for Modelling Hydraulic and Environmental Systems (IWS)*

Corresponding Authors: kevin.mumford@queensu.ca, wolfgang.nowak@iws.uni-stuttgart.de, anneli.guthke@iws.uni-stuttgart.de, colevandeven@eoas.ubc.ca, ishani.banerjee@iws.uni-stuttgart.de

Invasion percolation (IP) models, owing to their low computational effort requirement, have been used in several studies of multiphase flow in porous media 1, 2. Amongst them, many studies looked at gas flow in porous media 2–[4]. However, only a few studies have compared IP model simulation results to actual image or movie data from laboratory experiments. One reason for this might be the difficulty in quantitative assessment; IP models do not have a notion of experimental time but only have an integer counter for simulation steps that imply an order in time. The few existing experiments-to-model comparison studies have either used perceptual similarity 2, 5, [6] or spatial moments [4] as measures of comparison. On the one hand, comparison based on perceptual similarity is neither quantitative nor objective. Also, this procedure is tediously manual and consumes a lot of time, especially for experimental movies with many individual images, and for random-simulation models with many model realizations. On the other hand, comparison based on spatial moments suffers from a large loss of experimental information, since spatial moments are only a gross summary of the experimental images. Besides, there is no way to combine the information obtained from several spatial moments into a single goodness-of-fit metric.

In this work, we present a time-matched comparison method, which is both objective and quantitative. First, we perform a volume-based time matching between real-time experiments and IP model results. Then, we evaluate the quality of fit using a diffused version of the so-called Jaccard index. Being a measure of similarity between sets (e.g., in image analysis and object recognition), the Jaccard index is the size of the intersection divided by the size of the union of two sets. Here, these two sets are the gas-occupied volumes in experiment and simulation. Our diffused version of this metric is obtained by Gaussian blurring the experimental as well as the model images, using different extents of blurring. We demonstrate the applicability of our method on a laboratory-scale experimental movie of gas injection in homogenous, saturated sand [7], comparing it to the simulation results of an IP model (based on [4]) over many equiprobable realizations. The realizations vary in their initial entry pressure field. The reason for using many such equiprobable realizations is to capture the inherent pore-scale heterogeneity of the sand.

This method, being quantitative, is more objective than a perceptual comparison. It is also found to retain more detailed information in the data than spatial moments. As a result, it is a more reliable method for comparison. In contrast to the original Jaccard index, the diffused index enables to evaluate even model realizations with just a slight translation in space as a good fit. The most appropriate extent of blurring of the images is specific to the relevant scales of interest. The proposed metric can be further used for model calibration, model validation and inter-comparison of models. However, these applications are beyond the scope of the present study.

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1219

Modelling non-isothermal effects in a proton exchange membrane fuel cell (PEMFC)

Authors: Sagrario Muñoz[1]; V. María Barragán [1]

[1] *Department of Structure of Matter, Thermal Physics and Electronics, Faculty of Physics, Complutense University of Madrid*

Corresponding Authors: vmabarra@ucm.es, smsm@ucm.es

The knowledge of the heat flow in fuel cell is of great importance to predict its performance. The different energy rates that flows through each compartment causes a temperature gradient that leads to areas of excess heat. Thus, the assessment of the overall energy requirements is a decisive point to reach the goals of performance. Electromagnetic simulations have been proven as an adequate support for the previous performance of the fuel cells by designers and scientists and have become an important research field in recent years. Thus, it is feasible to predict and visualize the heat flow and the temperature gradient on a proton exchange membrane fuel cell (PEMFC).
This work aims at the modelling of a three-dimensional proton-exchange fuel cell by using COMSOL Multiphysics® software. Our PEMFC design considers as electrolyte the non-reiforced Nafion 117 membrane. The model includes besides the membrane, the MEA composed by two electrodes of platinum supported in carbon black and two gas diffusion layers (GDL) like carbon paper. This model was used to investigate the temperature gradient and the heat map. The results show remarkable differences in temperature of the different compartments of the fuel cell, showing the maximum values in the membrane region. The model was validated with the experimental results of the current-voltage characteristic measured at ambient temperature, and compare with the expected theoretical current-voltage curves for the corresponding isothermal fuel cell. The temperature gradient observed and the heat map might shed light to future studies of the performance of PEFFC under non-isothermal conditions that could lead to an undesired performance.

Acknowledgements
This work was supported by the Universidad Complutense of Madrid under the Project for Research Groups (Bioelectromagnetism Research Group 910305) and by Banco de Santander and Universidad Complutense of Madrid under the Project PR75/18-21589.

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Mechanism Study on the Influence of Low Salinity Water on Interface Characteristics of the Fluid and Rock

Author: Di Zhu[1]

Co-authors: Binfei Li [2]; Zhaomin Li ; Haifeng Li [3]

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

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

[3] *China Oilfield Services Limited*

Corresponding Authors: lizhm@upc.edu.cn, 1369300487@qq.com, libinfei999@126.com, 645213255@qq.com

Low salinity water flooding is a method for EOR through the injection of water with 1000-5000 mg/L of total dissolved solids(TDS). Low salinity water can improve the interface properties of crude oil, water and reservoir rocks. The addition of low salinity water in the process of reservoir development can change the oil-water interfacial tension and the wettability of reservoir rocks to promote the desorption of crude oil in the formation, so as to improve the displacement efficiency and oil recovery. In this paper, the effects of ion types and concentration on the properties of fluid and reservoir under the condition of low salinity water were investigated by the measurement of oil-water interfacial tension and the three-phase contact angle. And the effects of pH value on the interface were analyzed. The experimental results show that the oil-water interfacial tension gradually increases with the decrease of solution salinity, among which Ca^{2+} has the greatest influence on the oil-water interfacial tension and Mg^{2+} has the minimal effect under the experimental conditions. The interfacial tension between aqueous solutions of different ions and oil droplets increases more and more rapidly with the decrease of salinity and the gap decreases gradually. With the decrease of the pH value, the oil-water interfacial tension decreases significantly. Moreover, with the decrease of salinity, the contact angle of rock-oil-water becomes bigger, and the hydrophilicity of rock is enhanced. The three-phase contact angle shows the variation of 22.14° during the dilution process of simulated formation water under the experimental conditions. And with the pH value of low-salinity water increasing, the three-phase contact angle increases. In addition, the variety of the types and the salinity of anions have little influence on interfacial tension and three-phase contact angle. Under suitable conditions, the interface characteristics can be improved by the low salinity water imbibition-displacement, which has wide application prospects.

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A Hybrid-driven method to improve dynamical reservoir characterization

Author: Vanessa Simoes[1]

Co-authors: Horrara Diógenes [1]; Marianna Dantas [1]; Patrick Machado [1]

[1] *Schlumberger*

Corresponding Authors: hlima2@slb.com, vanessasimoes@gmail.com, msilva108@slb.com, pmachado3@slb.com

Petrophysical characterization includes the evaluation and integration of data from multi-disciplinary well logging measurements. As the different types of measurements present different depths of investigation and multiple physics, this data can provide information for multiple depths of investigations, which allows for a combined method sensitive to the radial water saturation from the wellbore to the virgin reservoir.
In Brazil, the comparatively lower hydrocarbon recovery factor in carbonate reservoirs represents one of the biggest challenges in production. For that reason, there is an increasing interest in improving the recovery factor and as part of this challenge, increasing the understanding of the properties that influence multiphase fluid flow including wettability and the connectivity of the pore network. Studying the near-wellbore region with the integration of logs and cores provides an opportunity of improving knowledge about fluid flow in situ conditions and enhancing the estimation of residual oil saturation, by better understanding the pore network system characteristics, which are important

parameters for reservoir characterization and simulation.
In water-based mud drilled wells, we observe a radial saturation profile, and it is crucial for log measurements that are sensitive to the pore saturation that the actual saturation is considered. This methodology is based on data and physics-driven methods to quantify near-wellbore water mud invasion, which is used to correct the traditional petrophysical estimation, improve the final hydrocarbon estimation, and provide an estimation of the minimum movable hydrocarbon fraction of the reservoir. This method is based on multi-physics analysis, fluid flow characterization, and a neural network trained machine learning method. The training and test datasets were developed using a reservoir model in an industry reference reservoir simulator covering a broad range of scenarios of interest. It is based on coupling the three different mechanisms multiphase: fluid Darcy's law, material balance equation, and capillary pressure. In the data-driven part, we trained a fast neural network to predict the radial fluid flow in the near-wellbore region with less than 1% error and when applied to field data it showed an agreement with combined logs and core data .
The final estimation includes the water saturation radial profile and the inverted residual oil saturation . To reduce the input proxy parameters for relative permeability and capillary pressure curves we adopted core and log calibrated Brooks-Corey equations.
The methodology has been applied to a complex carbonate field data with good agreement for core and logs measurement, which represents a validation for the methodology proposed.
Additionally, log measurements are sensitive to water saturation invasion varying from 1 inch to 50 inches away from the borehole wall, information that is essential to extract the radial profile using the methodology. We integrate multiple logs, petrophysical properties, and core measurements to provide the inputs to derive a calibrated water-based mud invasion profile around the borehole, together with a characterization of multiple formation properties.

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Hydrodynamic Dispersion in Simple Pore Geometries: Combining Experimental and Simulated Results at Individual Pore Scales

Author: Matthijs de Winter[1]

Co-authors: Kilian Weishaupt [2]; Stefan Scheller [3]; Stefan Frey [3]; Amir Raoof [1]; S. Majid Hassanizadeh [1]; Rainer Helmig [2]

[1] *Utrecht University*

[2] *University of Stuttgart*

[3] *Visualization Research Center, University of Stuttgart*

Corresponding Authors: smhfba@yahoo.com, steffen.frey@visus.uni-stuttgart.de, kilian.weishaupt@iws.uni-stuttgart.de, d.a.m.dewinter@uu.nl, a.raoof@uu.nl, rainer.helmig@iws.uni-stuttgart.de, stefan.scheller@visus.uni-stuttgart.de

Solute transport across porous media is a multi-scale process. Laws of physics describe the behavior at molecular to single-pore level while empirical relations describe macro scale behavior. We have studied an intermediate scale (micrometer –mm) by confocal scanning laser microscopy (CSLM) and computer simulations. Fluorescent colloids are transported across a microfluidic model made from PDMS and imaged by CSLM. The CSLM data is analyzed by micro-particle image velocimetry (micro-PIV) to derive vector maps. In a benchmark test, the combination of CSLM and micro-PIV produces mean velocities comparable quantitatively with the expected velocities based on the experimental conditions.

The next step is analyzing a larger, regular grid of pores. It is verified that experimental and simulated data are qualitatively equal. The flow direction varies across the pore grid because three sides of the grid are closed and so the flow has to enter and leave the pore grid through the same side. We show that the velocity profiles in the individual pores are all parabolic. However, by conducting a streamline analysis, we find that the time-of-arrival of solute travelling along different streamlines can vary significantly within a single pore. Although the structure is simple, the solute trajectories are very complex. With that observation we will discuss hydrodynamic dispersion in terms of 'streamline routing'and 'Brownian motion'.

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Performance Evaluation and Mechanism Analysis of Organic Clay Inhibitors with Low Molecular Weight

Author: Jingwen Wang[1]

Co-authors: Weian Huang [1]; Yu Fan [2]; Bo Zeng [2]; Haoyong Huang [2]

[1] *China University of Petroleum*

[2] *Shale Gas Research Institute, Petrochina Southwest Oil and gas field Branch*

Corresponding Authors: huang_hy@petrochina.com.cn, fanyu@petrochina.com.cn, zeng_bo@petrochina.com.cn, 17854227136@163.com, 20070067@upc.edu.cn

High shale content and low permeability formation is prone to water sensitive damage during water injection. Macromolecular clay inhibitor is easy to block the pore throat of low permeability formation, and makes the formation damage more serious. Application of organic clay stabilizer with low molecular weight has drawn more and more attention. The performance of 10 kinds of organic small molecular clay stabilizers, including one small molecular polyamine (1#), 4 types of small molecular cations (2~5#), 2 kinds of water-based cations quaternary ammonium salts (6~7#), one modified sugars (8#) and 2 types of choline chloride (9~10#), was evaluated by the static centrifugation method. Micromolecular clay stabilizers (9#, 6#, and 7#) were sorted and mixed. The anti-swelling rate of the combination system reached the highest of 87.88%, and the wash resistant rate reached 100%. The result of indoor core flow experiment showed that the combination system had better durable anti-swelling property. The particle size test and scanning electron microscope showed that organic low-molecular-weight clay stabilizer adsorbed on the clay particles and caused clay aggregation. The findings of Zeta potential test and interlayer spacing analysis illustrated that the clay stabilizer compressed the diffused double electric layers to reduce hydration repulsion and interlayer spacing, inhibiting clay swelling and dispersion. The study is helpful to optimize the clay inhibitor suitable for tight water-sensitive stratum and ensure the safety and efficiency of the process of water injection in low permeability oilfield.

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Contrast enhanced X-ray micro-tomography of tomato fruit tissues for microscale gas transport simulation

Authors: Hui Xiao[None]; Pieter Verboven[1]; Agnese Piovesan[2]; Bayu Nugraha[3]; Bart Nicolai[None]

[1] *KU Leuven - University of Leuven*

[2] *KU Leuven*

[3] *Bayu Nugraha*

Corresponding Authors: pieter.verboven@kuleuven.be, bayu.nugraha@kuleuven.be, hui.xiao@kuleuven.be, agnese.piovesan@kuleuven.be

Tomato, Solanum lycopersicum L., is one of the important fruit worldwide, both in volume of production and nutritional value. Tomato tissue is mainly composed of cells and intercellular pores. During maturation, tomato fruit require oxygen for respiration and produce carbon dioxide and ethylene for ripening. The structural composition of the fruit affects internal gas distribution, thus affecting fruit quality 1. Understanding the gas transport inside tomato fruit can help to improve ripening and storage conditions, thereby reducing losses during postharvest storage.
Compared with other bulky fruits (such as apple and pear), tomatoes are not homogeneous, and the pore microstructure in different tissue types will result in different gas transport patterns. For this reason, the 3D microstructure of different tomato tissues (including pericarp, septa, placenta and columella) were explored using X-ray micro computed tomography (u-CT). However, conventional X-ray micro-CT cannot clearly separate the individual cells in dense tissue fruits like tomato. According protocols developed in our lab 2, in this study, we applied 10 % cesium iodide solution to improve the contrast between the cells of different tissues of mature tomato fruit. The X-ray projection images were acquired by a Phoenix Nanotom micro-CT system (General Electric, Heidelberg, Germany) on a 12-bit 2304×2304 detector with voxel resolutions of 3.25 μm at 60 kV and 225 kA. Greyscale projection images were imported into Avizo 9.4 (VSG, Bordeaux, France) to generate binary images and segment single cells. Then, a microscale gas transport model was constructed for oxygen, carbon dioxide and ethylene diffusion at 18 ℃ to evaluate the effect of microstructure on effective tissue diffusivity. The microscale simulation results indicate different transport patterns for the three gases. Effective diffusivity values for different tissue types were obtained and explored with respect to the structural properties of the cells and pores in different tissue types.

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1226

Assessment of Geochemical Reactions in Porous Formation Compressed Energy Storage Systems

Authors: Chidera Iloejesi[1]; Lauren Beckingham[1]

[1] *Auburn University*

Corresponding Authors: coi0002@auburn.edu, leb0071@auburn.edu

In porous formations used for compressed energy storage, working fluids such as air, CO2, or H2, are injected into and extracted from the subsurface for energy storage or production based on energy demand. These systems are a promising means of abating the limitations of intermittent renewable energy production. In addition, the properties of CO2 under system conditions make it a favorable choice of working gas. However, cycling of CO2 in the subsurface creates conditions favorable for potential geochemical reactions in the subsurface that can influence formation properties and thus operational performance and safety. This work utilizes reactive transport simulations to evaluate the geochemical reactions between injected CO2 and the mineral facies of the Paluxy formation subjected to flow regimes resulting from operating a compressed energy storage plant for a four-months study period. The numerical simulation considers and compares injection only (uni-directional flow) and injection-extraction (bi-directional) flow systems corresponding the flow regime for CO2 sequestration and compressed energy storage, respectively. The result shows that the uni-directional flow simulation is dominated by mineral dissolution. The result of the bi-directional flow simulation shows that the influx of acidic and highly saturated brine solution into the core reduces the reaction driving force resulting in gradual mineralization of the injected CO2 that follows an initial mineral dissolution. The observed mineral evolution results in an increase in porosity from 24.84% to a uniform value of approximately 33.6% for the uni-directional flow simulation while the bi-directional flows has a porosity of 25.8% in the least porous grid cell and 31.1% in the most porous grid cell.

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Carbon Dioxide Plume in Bespoke 2D Porous Micromodels

Author: Niloy De[1]

Co-authors: Patrice Meunier [2]; Yves Méheust [3]; François Nadal [1]

[1] *Wolfson school of Mechanical and Electrical Engineering, Loughborough University, Loughborough, UK*

[2] *IRPHE, CNRS, Aix-Marseille University, France*

[3] *Laboratoire GéoScience, Université de Rennes, France*

Corresponding Authors: meunier@irphe.univ-mrs.fr, f.r.nadal@lboro.ac.uk, yves.meheust@univ-rennes1.fr, n.de@lboro.ac.uk

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In the current context of global warming, the short-term mitigation of greenhouse gas emission is of utmost importance. In this context, geological storage of carbon dioxide (CO_2) appears a promising solution. Upon injection, supercritical CO_2 rises up to the top caprock and immediately starts dissolving at the water/brine interface, leading to a CO_2 enriched layer of brine that happens to be heavier than the underlying pure brine. After a diffusion stage, this unstable configuration triggers a

gravitational instability where convective plumes are generated and pour downwards to the bottom of the aquifer. In such a convective regime, the dissolution rate of CO_2 - that is the efficiency of the CO_2 -trapping is greatly enhanced. However, the trapping efficiency is drastically affected by dispersion and mixing effects occurring at the porous scale [1, 2, 3].
In this work, experiments are performed to study the CO_2 plume migration by means of in-house built microfuidic micromodels (pseudo Hele-Shaw cells). The micromodel core is made of NOA-63, a UV curable photo resin which is impermeable to gases. We developed a soft-lithography repeatable protocol to make symmetric regular patterns of cylindrical pillars sandwiched between two vertical plane walls separated from each other by a 400 μm gap. Pillars diameters ranging from R = 200 to 400 μm and edge-to-edge distances (between pillars) ranging from R to 4R have been tested.
The water-filled micromodel was placed vertically in a CO_2 -pressurized chamber, and plumes were visualized using pH-sensitive colour indicators - since CO_2 -dissolution increases the acidity of aqueous solutions. We have used Bromocresol Purple (BP) whose color change region lies between 6.8 and 4.8 units of pH. The partial pressure of CO_2 ranging from 1 to 8 bar has been explored. we observed that lateral growth of the gravitational fingers is enhanced by porous dispersion, which in turn reduces transverse concentration gradients in the system. This leads to decreases the growth rate of the instability(for a given value of the permeability) and mitigates the dissolution rate of carbon dioxide - i.e. the quantity of CO_2 dissolved in the liquid per unit time (Sherwood number).

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1228

Permeability and Adsorption of Light Gas Through Mature Shale Kerogen by Molecular Simulations

Author: Fouad Oulebsir[1]

Co-authors: Romain Vermorel ; Guillaume Galliero

[1] *University of Pau*

Corresponding Authors: guillaume.galliero@univ-pau.fr, fouad.oulebsir@univ-pau.fr, romain.vermorel@univ-pau.fr

The profitability of shale reservoirs strongly depends on the quality, type and content of organic matter contained in the rock. Indeed, more than half of the hydrocarbons stored in the shale are adsorbed in the solid porous organic matter, the so called kerogen. The latter exhibits a microporous (porosity < 2nm) amorphous structure, and acts as both the source and the reservoir of hydrocarbons. Kerogen is finely dispersed in the mineral matrix of shale and represents about 5% of the total mass of the rock.

The understanding of the transport of hydrocarbons (permeability coefficients) at the microporous scale of shale systems and their storage capacities (adsorption quantities) is of crucial importance for optimizing the recovery of these resources. More specifically, how the structural properties of

the microporous shale kerogen and thermodynamic conditions influence its transport properties is very important especially for reserve estimation and their recovery plans.

However, hydrocarbon transport within kerogen micropores exhibits a non-Darcy behavior governed by molecular diffusion, which mainly arises from strong adsorption in kerogen.

In this work, we propose a numerical approach based on molecular dynamics and Monte Carlo simulations, performed on molecular models of mature kerogen. Supercritical thermodynamic conditions (high pressure, high temperature) typical of shale gas reservoirs were considered. More specifically, this work investigates the transport and adsorption properties of pure fluids (light alkanes) in mature kerogen structures reconstructed by molecular simulations. We focus on the dependence of the transport properties and storage capacities (adsorption) on thermodynamic conditions (pressure gradient at a fixed temperature) as well as the influence of the pore size distribution (aspect ratio between the pore size and the gas molecule diameter).

We will report estimates of the macroscopic porosity values of mature shale gas samples by means of adsorption isotherms computed by molecular simulations. Furthermore, our results evidence how transport mechanisms are different from those of meso/macro porous materials and highlight the impact of the porous structure and thermodynamics conditions. Actually, the tighter and the more tortuous is the porous network, the more activation energy phenomena dominate the flow mechanism.

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Application of Discrete Fracture Network Modeling using Sequential Gaussian Simulation

Authors: Timur Merembayev[1]; Yerlan Amanbek[2]; Sanjay Srinivasan[3]

[1] *International IT University, Almaty*

[2] *Nazarbayev University*

[3] *Pennsylvania State University*

Corresponding Authors: timur.merembayev@gmail.com, yerlan.amanbek@nu.edu.kz, szs27@psu.edu

Many flow and transport simulations through fractured media are widely used in various subsurface applications. The simulation of fracture geometry system using the geotechnical aspects requires large computational resources. In this work, we present the model of a fracture network system using the Sequential Gaussian Simulation (SGS) method 1. This method is based on the probabilistic approach to estimate the fracture network.
To simulate a fracture network, fractures statistics and a variogram model are required. We get this information from a zone where the behavior of fractures is known. In an unknown zone or in a zone where a fracture network needs to be simulated, we use the Poisson distribution to seed future fractures.
We propose the method which has two stages: the first stage is to search for the nearest fractures in the given segment of the propagation. A radius of the segment is determined by the lag value from the variogram of the known zone and the segment angle is a constant value. The second stage is to model an azimuth of the new fracture using the SGS method. All two stages of the method are calculated iteratively with termination conditions. We show numerical examples and comparisons of the simulated and realistic fractures from Kazakhstan and the United Kingdom. The verification was done by comparing the distribution of fracture angles for the original fracture networks and simulated fracture networks in the unknown area. We have observed similarities between the histograms for the original and simulated fractures. It was also verified by examining the concentration

at the production well using the incompressible flow and transport model through the simulated fracture network and the original fracture network. There is good agreement in both cases and in the breakout time.

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Study on multi-phase seepage of complex pore network in strongly heterogeneous carbonate reservoir based on various methods：A case study in Upper Cretaceous Khasib of the E Oilfield in the Middle East

Authors: Hao Lu[1]; Hongming Tang[1]; Yijun Wang[1]

[1] *College of Earth Science and Technology, Southwest Petroleum University*

Corresponding Author: homeluhao@163.com

The E oil field in the Middle East is a strong heterogeneous carbonate reservoir with billion ton reserves. The main oil-bearing layer Khasib consists of grainstone and packstone. The high permeability zone, dense clumps and strongly heterogeneous are the main factors affecting the development effect.

In this paper, the pore-throat distribution of complex pores network in the reservoir was characterized quantitatively by means of scanning electron microscopy and constant velocity mercury injection. The pore structure was reconstructed by computed tomography and digital core technology to visually analyze the pore connectivity. The influence of dominant channel and dense clumps on oil-water two-phase flow was characterized by magnetic resonance imaging and online nuclear magnetic resonance test. By employ the wettability and two-phase relative permeability tests, the displacement efficiency of different media were compared, and the effects of different parameters on oil seepage were analyzed combining with the dynamic theoretical curve of two-phase flow pressure.

The results show that there are various combinations of diverse pore types and pore throat sizes, such as intergrain pore, moldic pore and intrafossil pore. The micro dominant channel and dense clumps are the main reasons for the strong heterogeneity of reservoir. The pores in the packstone are relatively uniform, but small throat (2.0μm in average) of pores results in the poor connectivity and low average permeability (11.2mD, only 1/5 of that of grainstone). The packstone is oil-wet and its pore-throat structure is low permeability and fine throat, which results in high injection pressure and low pumping rate, with an average displacement pressure of 0.3MPa, which is 15 times that of grainstone. The dominant channel is the main factor leads to the water breakthrough during water flooding, and the dense clumps is the barrier that the remaining oil in the adjacent area cannot be migrated, both lead to low swept efficiency. The comparison of oil-gas and oil-water relative permeability shows that the residual oil saturation of core after nitrogen displacement is 25.3% lower than that of water displacement, and the displacement efficiency is increased by 46%. The theoretical chart verifies that the pressure drop of gas model is less than that of water displacement model, which can maximize the usage of displacement energy.

Through the study, the complex pore structure and multiphase seepage mechanism of the reservoir in E oil field are clarified. It is proposed that reservoir stimulation and nitrogen displacement are effective approaches to solve the poor connectivity and low displacement efficiency, which could provide support for the formulation of oilfield development policy and reference for the development in adjacent areas.

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Pore-Scale Imaging of Controlled-Salinity Waterflooding in a Heterogeneous Carbonate Rock at Reservoir Conditions

Author: Ahmed Selem[None]

Co-authors: Nicolas AGENET [1]; Ying Gao [2]; Qingyang Lin [2]; Ali Qaseminejad Raeini [3]; Martin Blunt [2]; Branko Bijeljic [4]

[1] *TOTAL S.A.*

[2] *Imperial College London*

[3] *Research Associate*

[4] *Imperial College*

Corresponding Authors: b.bijeljic@imperial.ac.uk, a.qaseminejad-raeini09@imperial.ac.uk, y.gao15@imperial.ac.uk, m.blunt@imperial.ac.uk, nicolas.agenet@total.com, q.lin11@imperial.ac.uk, a.selem18@imperial.ac.uk

Controlled salinity water-flooding (CSW) is a promising enhanced oil recovery technique, yet the pore-scale mechanisms that control the process remain poorly understood especially in carbonate rocks. The aim of this experimental study is, therefore, to gain novel insights into CSW by elucidating the impact of wettability on oil displacement in the complex pore space of carbonates. X-ray imaging combined with a high-pressure high-temperature flow apparatus was used to image and analyse in situ CSW in an Estaillades limestone core sample (5.9 mm in diameter and 10 mm in length).

Firstly, we characterised the pore space by differential X-ray imaging with a voxel size of 2.9 μm with which we measured resolved porosity (12.8%) and sub-resolution micro-porosity (17.1%). Next, to establish the wettability conditions found in oil reservoirs, the Estaillades sample was aged for three weeks at 11 MPa and 80℃. The weakly oil-wet sample was then flooded by injecting low salinity brine at a range of increasing flow rates, namely at 1, 2, 4, 11, 22 and 42 μL/min. Tomographic images were acquired after each flow rate. A total of 60 pore volumes of low salinity brine were injected recovering 86% of the oil initially in place in resolved macro-pores.

Furthermore, in situ geometric contact angles and brine-oil curvatures were measured to characterize wettability changes within the pore space. Moreover, a generalized pore network extraction algorithm was utilised to investigate and map the pore and throat fluid occupancy to assess how injection altered the pore-scale fluid configurations. Both measured geometric contact angles and mean curvatures showed a shift from a weakly oil-wet towards a mixed-wet state as more pore volumes of low salinity brine were injected into the sample. The mean contact angle value decreased from 124° before the start of low salinity water injection to 107.7° at the end. The measured mean curvature and the associated capillary pressure values were negative. The capillary pressure increased towards zero, as the wettability progressed towards a mixed-wet state with low salinity injection,

The pore and throat occupancy analysis revealed a change in fluid distribution in the pore space. Low salinity brine initially invaded large pores, but as more brine was injected the fraction of small pores and throats occupied by oil decreased and an equal fraction of large pores and throats were

occupied by both oil and brine. This change in fluid occupancy is a clear indication of an alteration in the rock wettability.

Overall, our analysis shows that wettability alteration towards a mixed wet system caused by low salinity brine was the main mechanism for increased oil recovery. The same methodology for wettability characterisation on a pore-by-pore basis can be applied to study displacement in mixed-wet porous media in other applications, such as carbon dioxide storage, batteries and packed bed chemical reactors.

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A deformation-dependent permeability model for polycrystalline rocks

Author: Florian Zill[1]

Co-authors: Olaf Kolditz [2]; Thomas Nagel [3]

[1] *Helmholtz Centre for Environmental Research UFZ*

[2] *Helmholtz Centre for Environmental Research UFZ / TU Dresden*

[3] *Technische Universität Bergakademie Freiberg*

Corresponding Authors: olaf.kolditz@ufz.de, florian.zill@ufz.de, thomas.nagel@ufz.de

In order to achieve the goal of the Paris Climate Agreement and to reduce CO₂ emissions, renewable energies are mandatory. Their volatile nature necessitates the expansion of energy storage systems. Underground caverns for storing energy sources –so far mainly natural gas or compressed air –offer a promising option. The storage of hydrogen produced from renewable sources can improve the use of volatile renewable energies.

To ensure long-term stability of cavern storage systems, simulations are used to predict material behaviour and, if necessary, adapt the operating framework to a safe state. Caverns for energy storage are usually build in salt deposits underground due to the favorable low permeability of the rock salt. The material model plays a central part in the simulation. Salt rock behaves in an elastic-viscoplastic way and was tried to be depicted in an accurate way by different models in the past. A crucial detail regarding the tightness of cavern boundaries is the effect of fluid infiltration into the grain boundaries of the host rock, which consequently influences the stability.

Expanding on the work of Olivella and Alonso (2008) a deformation-dependent permeability model for polycrystalline material is developed, based on embedding fractures in finite elements. The model is numerically implemented in the open source multiphysics simulation framework OpenGeoSys (Kolditz et al., 2012; Bilke et al., 2019). Using the hydromechanical process, which relies on the theory of porous media, the model is validated with multiple benchmarks and tested against experimental data from percolation experiments on rock samples (Kamlot, 2009).

The simulation results demonstrate the ability of the model to produce anisotropic behaviour as well as quasi-isotropic behaviour. Modeling and simulating the percolation experiment showed that our model reproduces the same preferential directions of the infiltrating fluid and can match the pressure and time at fluid breakthrough. In comparing simulations with parameter variations, the influence of each parameter of the model is shown. These promising results indicate that the permeability model may prove useful in depicting the fluid infiltration effect in cavern simulations and will be further developed to account for plastic effects.

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The effect of buoyant convection on the buoyancy-driven spreading and draining that arises within a layered porous media with a permeability jump

Author: Md Imran Khan[1]

Co-authors: K. S. Bharath [1]; M. R. Flynn [1]

[1] *University of Alberta*

Corresponding Authors: mrflynn@ualberta.ca, mdimran@ualberta.ca, kattemal@ualberta.ca

We investigate theoretically the impact of introducing convective instabilities along the sc-CO_2/acid gas-groundwater interface in a saturated, layered porous aquifer with a sloping permeability jump. Particular emphasis is placed on the time varying nature of the (miscible) sc-CO_2/acid gas plume in the post injection phase for three different dissolution models namely: constant dissolution, dissolution with simultaneous shutdown and finally, dissolution with sequential shutdown. To study the effect of these hydrodynamic instabilities on the dynamics of the porous media plume, we apply a sharp interface model and analyze the impact of the dissolution models as well as geometric parameters on the front speeds of the gravity currents that propagate up- and downdip along the permeability jump. Also of interest is to estimate the fraction of the injectate that propagates up- vs. downdip and the intermediate and long term run-out lengths of the gravity currents. To gauge the effectiveness of dissolution as a long-term trapping mechanism, we consider the temporal evolution of the storage efficiency and examine the impact of changing the dissolution strength; and the shutdown onset time, t_1 and e-folding decay time, t_2 for simultaneous vs. sequential shutdown. Solutions show that in case of a lower layer of infinite depth, the up- and downdip migration distance falls with increasing dissolution strength, which stems from the lower proportion of fluid discharged by the vertical plume that can flow along the permeability jump. This is true across all dissolution models and shutdown regimes that we investigate. For special cases with increased values of t_1, as the shutdown regime is achieved, the previously-arrested gravity currents are able to remobilize. Furthermore, delaying the onset for shutdown and increasing the decay time drastically reduce the gravity current front speeds while increasing the aggressiveness with which shutdown is achieved.

Consequently, all three dissolution models show higher long-term storage efficiencies. The constant dissolution model gives the highest long term storage efficiencies, followed by sequential shutdown and simultaneous shutdown models. A more general comparison between models reveals regions of the parameter space where horizontal mixing in the ambient fluid plays a dynamically significant vs. insignificant role.

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Scale-effect in the simulation of two-phase flow in porous media

Author: Brandon Yokeley[1]

Co-authors: Behzad Ghanbarian [1]; Muhammad Sahimi [2]

[1] *Porous Media Research Lab., Department of Geology, Kansas State University*

[2] *University of Southern California*

Corresponding Authors: moe@usc.edu, yokeleyba@ksu.edu, ghanbarian@ksu.edu

Two-phase flow in porous media is important to a broad range of applications from hydrology and petroleum engineering to sequestration of CO2 in rock formations and evaporation of brine in soils. It is well documented in the literature that soil hydraulic and rock petrophysical properties are scale dependent. Although the concept of representative elementary volume (REV) was developed for determining the minimum size of the system to which macro-scale transport and flow equations are applicable, it was mainly based on single-phase permeability. In this study, we investigated the effect of scale on water and oil relative permeability curves via pore-network models. We computed the relative permeability curves with various network sizes, assuming either strongly or intermediately water-wet pore space that were constructed with various pore-throat and pore-body size distributions. In all the pore networks, the coordination number was set equal to six. The size distributions of pore throats and pore bodies were taken to be a truncated Weibull probability density function that represents a relatively wide range of pore-scale heterogeneity. The results indicate that the oil relative permeability curves manifest greater variations and scale dependence when compared to the water relative permeability, particularly when the network sizes are small. We also found that as the pore-throat size distribution became broader, making pore-scale heterogeneity stronger, the oil relative permeability REV must be also larger. However, the REV for water relative permeability did not change significantly and was found to be the smallest when compared to that of the oil relative permeability, whereas the single-phase REV was the largest. This indicates that the water relative permeability is least affected by the scale and network heterogeneity in strongly and intermediately water wet systems. However, further investigations based on a broader level of pore-scale heterogeneity may still be required to confirm our initial findings.

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Transport and deposition of suspended particles in the context of permafrost thaw: An experimental and numerical modelling study

Author: Madiha Khadhraoui[1]

Co-authors: John Molson [1]; Najat Bhiry [2]

[1] *Département de géologie et de génie géologique, Université Laval, Québec, Canada*

[2] *Département de géographie, Université Laval, Québec, Canada*

Corresponding Authors: john.molson@ggl.ulaval.ca, madiha.khadhraoui.1@ulaval.ca, najat.bhiry@cen.ulaval.ca

Investigating the behavior of the mobile solid phase in porous media is important because particle migration during flow plays a determining role in soil stability, pollutant transport and loading of surface water from groundwater discharge particularly in northern areas where natural risks are amplified. Changes occurring during detachment of particles from the soil matrix and transport in the pore water can be difficult to study however, because they are evolutionary processes and depend on several parameters.

In order to investigate particle transport during permafrost thaw, laboratory column experiments were carried out under constant flow conditions and continuous injections of particle suspensions. Porous media heterogeneity was included using different grain size distributions. Spatio-temporal evolution of the hydraulic properties and soil porosity associated with the injected suspensions was studied using X-ray computed tomography imaging (CT-Scan), acquired before, during and after injections.

A simulation strategy is then proposed based on an analytical solution and a finite element numerical model. For velocity-dependent particle transport and deposition, we adopted the numerical model BIONAPL/3D for groundwater flow, advective-dispersive transport, and deposition of suspended particles through a porous medium.

Our simulations highlight the roles of hydraulic conditions and physical soil characteristics on particle transport and deposition mechanisms in porous media. The deposition kinetics and the hydrodynamic dispersion coefficients are controlled by flow velocity and the grain size distribution. Direct observations from X-ray imaging shows that the time-dependent changes in soil parameter distributions strongly depend on the concentration of the injected suspended particles.

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Quantification of non-linear multiphase flow in porous media

Authors: Yihuai Zhang[1]; Branko Bijeljic[2]; Ying Gao[1]; Qingyang Lin[1]; Martin Blunt[1]

[1] *Imperial College London*

[2] *Imperial College*

Corresponding Authors: y.gao15@imperial.ac.uk, m.blunt@imperial.ac.uk, q.lin11@imperial.ac.uk, yihuai.zhang@imperial.ac.uk, b.bijeljic@imperial.ac.uk

We measure the pressure difference during two-phase flow across a sandstone sample for a range of injection rates and fractional flows of water, the wetting phase, during an imbibition experiment. We quantify the onset of a transition from a linear relationship between flow rate and pressure gradient to a non-linear power-law dependence. We show that the transition from linear (Darcy) to non-linear flow and the exponent in the power-law is a function of fractional flow. We use energy balance to accurately predict the onset of intermittency for a range of fractional flows, fluid viscosities and three rock types, reconciling several literature datasets.

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Pore connectivity characterization of Woodford Shale using liquid imbibition and tracer gas diffusion methods

Author: Chen Zhao[1]

Co-authors: Qinhong Hu [1]; Qiming Wang [1]; Jing Zhang [2]; Roger Slatt [2]

[1] *University of Texas at Arlington*

[2] *The University of Oklahoma*

Corresponding Authors: chen.zhao3@mavs.uta.edu, qiming.wang@mavs.uta.edu, maxhu@uta.edu

Pore connectivity is an important index in reservoir characterization in the oil & gas industry due to its restrictive effects on liquid- and gas-phase transport and hydrocarbon recovery. With the ongoing rapid development of unconventional reservoirs, it is essential to study the pore connectivity of nanoporous shale for enhanced recovery of hydrocarbon production. This work aims to evaluate the pore connectivity of Woodford Shale, which include nine outcrop samples from south Oklahoma with different lithologies, by spontaneous imbibition (SI) and tracer-gas diffusion tests. Percolation theory has been applied in recent decades to describe fluid flow affected by rock's pore connections. The pore connectivity can be quantified and compared with the percolation threshold by the fluid imbibition behavior in SI 1. The 24 hrs 1-D co-current SI was performed on 1-cm3 cubic samples with deionized water 2. In conjunction with the SI work, tracer-gas diffusion was carried out to quantify the diffusion coefficient (Dp) of samples 3. Tracer-gas diffusion was conducted on 1-inch-diameter core plugs under three water saturation conditions: oven-dried; equilibrium-moistened in the humidity chamber with RH value of about 99%; and fully water-saturated. The samples exhibiting a good pore connectivity in SI tests show a decreasing Dp value with an increasing water content. The poorly-connected samples in SI tests have relatively stable Dp values with various water contents. All the results show that SI and tracer-gas diffusion tests could reasonably evaluate the pore connectivity of nanoporous shales.

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Fully-implicit dynamic pore-network modeling of two-phase flow in porous media

Author: Sidian Chen[1]

Co-authors: Chaozhong Qin [2]; Bo Guo [1]

[1] *University of Arizona*

[2] *Chongqing University*

Corresponding Authors: boguo@arizona.edu, sidianchen@email.arizona.edu

Dynamic pore-network modeling (PNM) has been widely used to model multiphase displacements in porous media. Prior numerical algorithms for dynamic PNM such as IMPES (implicit pressure explicit saturation) and IMP-SIMS (implicit pressure semi-implicit saturation) are only numerically stable or accurate for some flow regimes—characterized by the capillary number Ca and fluid viscosity ratio $\mathcal{M}$ (injected fluid over displaced fluid). Here we first perform a comprehensive analysis of IMPES and IMP-SIMS and then present a novel fully-implicit (FI) framework to address their limitations. We found that the numerical stability of IMPES is sensitive to the selection of the local capillary pressure function for each pore body. While previous IMPES algorithms were reported numerically unstable for low Ca flow, our implementation—using a smooth local capillary pressure curve for each pore body—appears numerically stable. Example simulations showed that while IMPES can precisely match with quasi-static solutions at equilibrium states, IMP-SIMS deviates from quasi-static solutions. The deviation of IMP-SIMS was found sensitive to the selection of pore geometries. We have tested cubic and square tube-type pore bodies. The deviation, though relatively small when cubic pore bodies are used, becomes more significant for square tube-type pore bodies. In addition, both IMPES and IMP-SIMS have mass conservation errors that are also sensitive to the selection of pore geometries. When cubic pore bodies are used, the mass conservation errors are negligible. However, when square tube-type pore bodies are used, the errors become much greater (up to 30% for IMPES and 45% for IMP-SIMS) especially for unfavorable displacements ($\mathcal{M} < 1$). Conversely, the new FI algorithm provides robust solutions for a wide range of flow regimes including near quasi-static flow ($Ca \to 0$) and an $\mathcal{M}$ that spans 0.01 to 10 for both cubic and square tube-type pore bodies. An exact match between FI and quasi-static solutions and exact mass conservation are observed for all simulations. Overall, the FI method provides a robust framework to study complex two-phase flow and transport problems at the pore scale.

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Buoyant convection from a discrete source in closed vs. leaky porous media

Authors: Morris Flynn[1]; Chunendra K. Sahu[2]; Mark Roes[1]

[1] *U. Alberta*

[2] *University of Cambridge*

Corresponding Authors: mroes@ualberta.ca, cks34@cam.ac.uk, mrflynn@ualberta.ca

The application of turbulent plume theory in describing the dynamics of emptying filling boxes, control volumes connected to an infinite exterior through a series of openings along the upper and lower boundaries, has yielded novel strategies for the natural ventilation of buildings. Making the plume laminar and having it fall through a porous medium yields a problem of fundamental significance in its own right, insights from which may be applied, for example, in the geological sequestration of acid-gas. After reviewing the theory appropriate to (rectilinear) plumes in porous media, we demonstrate how the model equations may be adapted to the case of an emptying filling box. In this circumstance, the long-time solution consists of two ambient layers, separated by a thick interface, where each layer has a uniform density. These lower and upper layers comprise fluid that is respectively discharged by the plume and advected into the box through the upper opening. Our theory provides an estimate for both the height and thickness of the associated interface in terms of, for example, the source conditions, the outlet area and permeability, and the dispersion coefficient,

The possibility of a steady state solution disappears if the bottom boundary is made to be impermeable. In this circumstance, contaminated fluid (i.e. fluid discharged by the plume) continues to accumulate in an ever-deepening layer along the bottom of the control volume. By adapting the steady state theory, a (nontrivial) prediction can be derived for the rate at which the control volume fills with this contaminated fluid.

Both of the above theories are corroborated with reference to experimental measurement. Experiments are performed under ambient pressures and temperatures and employ salt water plumes falling through water-saturated bed packs. Our experiments consider as independent variables the porous medium bead diameter and the plume source volume flux and reduced gravity. Generally favorable agreement between theory and experiment is found.

The talk will conclude with an assessment of the prospects for using a so-called filling-box model in describing some of the dynamics of acid-gas sequestration. Parallels to other geophysical flows that have likewise employed filling box models shall be drawn and briefly discussed.

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Review and Comparison of Numerical Strategies to Estimate the Full Permeability Tensor of Anisotropic Materials From Micro-Tomography Images

Authors: Hermes Scandelli[1]; Jean Lachaud[2]; Azita Ahmadi[1]

[1] *ENSAM - I2M*

[2] *University of Bordeaux - I2M*

Corresponding Authors: azita.ahmadi@ensam.eu, jean.lachaud@u-bordeaux.fr, hermes.scandelli@ensam.eu

X-ray computed micro-tomography (CMT) and direct pore-scale simulations are increasingly being used to estimate the permeability of porous media 1. However there is still confusion on the numerical strategy to define and the set of boundary conditions to enforce. We have identified five different numerical approaches in the literature and we have implemented them in the OpenFoam numerical framework. In order to be as generic as possible, different possible configurations for the boundary conditions were considered. The purpose was to determine the most suitable strategy to compute the full permeability tensor for a real non-periodic porous medium geometry and the set of boundary conditions with the least impact on the result. To this end, we have compared all the defined strategies against reference solutions for creeping flows (Darcy regime) on idealized geometries (sphere and cylinder arrays). Only one of the five methods has been proven to be rigorously correct in the general case of non-periodic anisotropic porous media. This strategy was then applied to a 3D CMT of Carcarb, a carbon fiber preform used as thermal protection in space vehicle heat shields. Strong attention has been put on the mesh convergence analysis. In this presentation we are going to address all these aspects, while explicitly detailing the calculation process leading to the determination of the permeability tensor and its extension to the weak inertial regime (Forchheimer correction) 2. The study concludes with direct observations of flow behaviors (streamlines) when inertial effects appear. They allow the identification of the proper characteristic length of the domain to be used in the Reynolds number to determine the flow regime.

The numerical framework that was developed during this study is made available in the Porous material Analysis Toolbox based on OpenFoam (PATO) released Open Source by NASA 3 (www.pato.ac).

Keywords: Porous media; Permeability tensor, Boundary condition configurations; Micro-tomography; Pore-scale numerical simulations; Characteristic length of the domain

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The Impact of Entrapped Air on Satiated Hydraulic Conductivity of Coarse Sands Interpreted by X-ray Microtomography

Authors: Tomas Princ[1]; Helena M.R. Fideles[2]; Johannes Koestel[3]; Michal Snehota[1]

[1] *Czech Technical University in Prague, Faculty of Civil Engineering*

[2] *Universidade Federal do Rio de Janeiro, Laboratório de Métodos de Modelagem e Geofísica Computacional*

[3] *Swedish University of Agricultural Sciences, Department of Soil and Environment*

Corresponding Authors: michal.snehota@fsv.cvut.cz, john.koestel@slu.se, tomas.princ@fsv.cvut.cz

The relationship between entrapped air content (ω) and the corresponding hydraulic conductivity (K) was investigated experimentally for two coarse sands (Princ et al., 2020). Additionally the pore-network model based on OpenPNM platform was used to attempt simulation of a redistribution of the air bubbles after infiltration.
Two packed samples of 5 cm height and 7.2 cm diameter were prepared for each sand. The cycles of infiltration and drainage led to entrapping of the air. The value of K was determined using Darcy's law by repetitive falling-head infiltration experiments. The entrapped air content was determined from gravimetrically after each infiltration run. The amount and distribution of air bubbles were quantified by X-ray computed tomography (CT) for selected runs. The obtained $K(\omega)$ relationship agreed well with Faybishenko's (1995) formula. CT imaging revealed that entrapped air contents and bubbles sizes were increasing with the height of the sample. This result was compared with the result from pore-network model. It was found that the size of the air bubbles and clusters increased with each repetition of the experimental cycle. The relationship between initial and residual gas saturation was successfully fitted with a linear model.
The combination of X-ray computed tomography and infiltration experiments has a potential to explore the effects of entrapped air on water flow.

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Application of Seismic Sedimentology in Reservoir Prediction: Taking Chenguanzhuang Area as an Example

Author: Zongwei Zhang[1]

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

Corresponding Author: 595975536@qq.com

Since the rise of seismic sedimentology, it has been widely used in thin sand body identification, sedimentary facies characterization, and reservoir prediction, and has achieved good results. In this paper, based on the seismic sedimentology method, taking the fourth lower section of the Chenguanzhuang Sha in the southern gentle slope of Dongying Sag as an example, the isochronous stratigraphic framework of the study area is established by analyzing the cycle characteristics and time-frequency characteristics of the study area; the sedimentary structure and logging response are analyzed to establish Three deposition modes; using 90° phase conversion, stratigraphic slicing technology, and fault-control sand fault zone elimination methods, carrying out research on thin sand bodies with complex fault blocks, identifying thin sand bodies, sedimentary facies types and planar deposition under the guidance of deposition modes Portrayal. The study found that there is a good correspondence between the datum cycle and the time-frequency characteristics. Two lower sand groups in the fourth member of the Shahejie Formation can be used for isochronous formation identification and interpretation; mudstones have high gamma and low wave impedance, and sandstones have low gamma The high wave impedance makes the amplitude a parameter indicating lithology. After the 90° phase conversion of seismic data, the valley is partial to the sandstone facies, which improves the interpretability of seismic data; under the guidance of the sedimentary model, analysis and interpretation of stratigraphic slices; fault zones The elimination of the inner surface improves

the visualization of the plane; the lower section of the fourth member of the Shahejie Formation in the Chenguanzhuang area is bounded by the Tong 4 fault, and the sand body is more developed in the south than in the north. The first sand group mainly develops shallow water delta sediments and lakeside dam facies sediments, including diversion Types of rivers, sand flats, beach dams, etc.; Ersha Formation developed Manhu niping, sand flats, mixed flats and beach bar deposits, clarifying the type of sedimentary facies, and providing guidance for the next exploration direction.

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Pore-scale flow with the memory-efficient Lattice Boltzmann formulation

Authors: Maciej Matyka[1]; Michał Dzikowski[2]

[1] *University of Wrocław, Faculty of Physics and Astronomy*

[2] *ICM, Interdisciplinary Centre for Mathematical and Computational Modelling, Warsaw University*

Corresponding Authors: m.dzikowski@icm.edu.pl, maciej.matyka@uwr.edu.pl

To effectively compute porous media properties based on the pore-scale modeling one needs to allocate enough computational power and memory to maintain large numerical samples. One of the common numerical methods used in pore-scale modeling is the Lattice Boltzmann Method (LBM).

Here, the LBM algorithm is simplified by assuming constant numerical viscosity (the relaxation time is fixed at $\tau = 1$). This leads to the removal of the distribution function from the computer memory. To test the solver the Poiseuille and Driven Cavity flows are simulated and analyzed. The error of the solution decreases with the grid size L as L^{-2}. Compared to the standard algorithm, the presented formulation is simpler, shorter in implementation, less error-prone and needs significantly less working memory in low Reynolds number flows. Moreover, we show that by expanding the multirelaxation time LBM scheme for tau=1 we gain significant speedup in the single component multiphase LBM if compared to standard algorithm. We test the implementation of the solver in TCLB code and simulate the fluid flow through a porous medium sample at the pore scale.
The talk will summarize and extend the results presented in https://arxiv.org/abs/1912.09327

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Maciej Matyka, Memory-efficient Lattice Boltzmann Method for low Reynolds number flows, https://arxiv.org/abs/1912.09

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Modeling the effect of microscale heterogeneities on soil bacterial dynamics and the impact on soil functions

Authors: Simon Zech[1]; Alexander Prechtel[1]; Nadja Ray[1]

[1] *Friedrich-Alexander Universität Erlangen-Nürnberg*

Corresponding Authors: ray@math.fau.de, simon.zech@fau.de, prechtel@math.fau.de

There is still no satisfactory understanding of the factors that enable soil microbial populations to be as highly diverse as they are. Mathematically based modeling can facilitate the understanding of their development and function in soils, e.g. with respect to habitat and carbon cycling.
Our mechanistic model is based on [1, 2] and allows studying the spatiotemporal dynamics of bacteria in unsaturated soil samples. In this presentation, different levels of saturation are investigated, for which the fluid (liquid and gas) distributions are calculated according to a morphological model similar to 3. As in [4], various bacteria strains and organic matter are heterogeneously distributed in CT scans of various soil samples.
The bacteria strains grow based on Michaelis-Menten kinetics due to the uptake of oxygen and dissolved organic carbon (DOC) present in the liquid phase. The development of bacterial colonies is realized in a cellular automaton framework (CAM) as presented in [1, 2] and going back to the work of 5. DOC is either present as a carbonaceous solution or hydrolized by a first order kinetics from heterogeneously distributed particulate organic matter (POM) sources. The diffusion of both nutrients oxygen and DOC are described by means of reactive transport equations, which include a Henry condition for the transfer from/into the gas phase. We apply the local discontinuous Galerkin (LDG) method as a discretization scheme.
Our simulations show that the impact that heterogeneity in nutrient and bacteria distribution has on overall biodegradation kinetics strongly depends on the scale of interest. On the scale of soil microaggregates (<250 µm) only very specific cases can be distinguished, e.g. when nutrient sources are isolated from bacteria due to a disconnected liquid phase. Furthermore, the biodegradation kinetics in the case of homogeneously distributed DOC, which corresponds to the state of a soil after a sudden flush of nutrients, e.g. by a fertilizer, differs significantly from the case of aggregated organic matter in form of POM.
However, on larger scales (millimeter scale), such heterogeneities have a large impact, as was shown in [6]. We conclude that the heterogeneous spatial structure must be resolved scale-dependently. Similar to [7], we include this information into a macro-scale model and estimate the overall CO2 production rate for different soil profiles.

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Numerical Simulation of CO2 enhanced gas recovery (CO2-EGR) for the optimal CO2 injection perforation position and injection rate

Authors: Liu Shuyang[1]; Sun Baojiang[1]

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

Corresponding Authors: sunbj1128@126.com, shuyang_liu@126.com

CO2 mitigation is urgently needed due to a large amount of CO2 emissions released by consumed massive fossil fuels, causing the global warming and other extreme weathers. As one of the promising technology of carbon capture, utilization and storage (CCUS), CO2 enhanced gas recovery (CO2-EGR) can sequestrate CO2 into the underground porous media and simultaneously exploit more clean natural gas from the depleted gas reservoir. The perforation position of CO2 injection well and injection rates play key roles to the natural gas recovery of CO2-EGR applications. Hence, in this work, the displacement behavior of natural gas by CO2 in the underground porous media was studied by carrying out the CO2-EGR simulation in a depleted natural gas reservoir. The perforation positions of CO2 injection were simulated at the bottom, middle and top layers of the reservoir model. The results shows that the top layer of the reservoir was the optimal position for the perforation of CO2 injection, and the reason should be the gravity effect. The gravity effect accelerated the vertical downward displacement of natural gas by CO2 and contributed to produce additional natural gas. Moreover, an optimization method was built by integrating genetic algorithm (GA) and TOUGH2 for obtaining the optimal injection rate. The optimal injection rate of CO2 was determined as 0.0824 kg/s while the perforation was set at the top layer of the reservoir, and the final natural gas recovery achieved up to 65.37%. This work may provide some insight for the CO2-EGR employment in the depleted natural gas reservoirs.

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Reactive transport in porous media: Modeling electro-diffusion process using Nernst-Planck-Poisson Equation

Authors: Sara Tabrizinejadas[None]; Jerome Carrayrou[None]; maarten saaltink[None]; Marwan Fahs[None]

Corresponding Authors: sara.tabrizi-nejad-as@etu.unistra.fr, jerome.carrayrou@unistra.fr, maarten.saaltink@upc.edu, fahs@unistra.fr

Many modern codes have been extensively used to describe reactive transport in different industrial and environmental applications. Most of these reactive transport codes neglect the columbic interactions between the charged particles and consider the Fick's law for the description of the diffusion processes. Fick's law assumes a constant diffusion coefficient for each dissolved species and this misleads to assuming that movements of each dissolved species in a system is merely based on the gradient of concentration. However, in reality, in a multicomponent electrolyte solution, each individual dissolved species can migrate differently according to its own ionic properties such as charge, ionic size or ionic mobility. This process is called electrochemical migration.

Recent studies prove that electrochemical migration processes have significant influence on the mixing of dissolved species. Existing studies on electrochemical migration are based on the null current assumption. This requires a departure from Fick's law by including an electro-diffusion coefficient that can be expressed in terms of charges and concentrations of chemical components via the Nernst-Planck equation. The null current assumption has a great advantage as it allows for simplifying the mathematical model by eliminating the Nernst-Planck equation. This simplification is highly important because it brings more convenience for including electrochemical migration processes in existing reactive transport models. In this case, this can be simply implemented by including an additional diffusion coefficient.
The null current assumption-based models limit the ability of the model to describe a domain subjected to an external field where the total electric field is affected by both internal interactions of ions and external applied electric field. Even without external electrical field, the validity of the null current assumption could be questionable. This topic has never been investigated in the past. The main goal of this work is to address this gap. We aim at evaluating the validity of the null current assumption and understanding its effect on reactive transport processes.
Thus, we introduce a new reactive transport model that allows for an accurate representation of the electrochemical migration processes without the null current assumption. The developed model is based on the advection-diffusion-reaction equations for describing transport processes and the Nernst-Planck and Poisson equations (NPP) for electrochemical migration processes. Transport and NPP equations are coupled together because in the Poisson equation, the electric field is linked to the total ionic concentration of species in the system. These coupled equations are solved using the finite element in COMSOL Multi-physics. We also implement with COMSOL a model based on the null current assumption. The fully coupled approach (i.e. one step approach) is applied to avoid numerical artifacts related to operator splitting. The new developed models (with and without null current assumption) have been validated using several benchmarks and by comparison with published works (e.g. Rasouli et al. 2015). We compare these models in several configurations of reactive transport. Our results show that in the case of high sorption rate, the null current model is no longer valid. The sorption leads to a significant departure between the models.

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Modelling biofilm formation in porous media flow

Author: Christoph Lohrmann[1]

Co-authors: Kartik Jain [2]; Christian Holm [1]

[1] *University of Stuttgart, ICP*

[2] *University of Twente*

Corresponding Authors: k.jain@utwente.nl, holm@icp.uni-stuttgart.de, clohrmann@icp.uni-stuttgart.de

Biofilms are colonies of sessile bacteria attached to surfaces. In many cases, they are encountered in complex, porous geometries where an external flow is present. They can be detrimental, *e.g.* in filtration systems, or beneficial, *e.g.* for microbially induced carbonate precipitation (MICP). In any case, the interplay between biofilm growth and external flow in confined geometries needs to be understood, starting at the pore scale.
We present a bacterial model based on a coupling between single cells and a surrounding flow. Bacteria are simulated as molecular dynamics particles, the fluid dynamics problem is solved via the lattice Boltzmann method. The two algorithms are connected via a point-friction coupling.
Starting with freely swimming cells, we are able to determine likely locations for biofilm initiation by explicitly taking into account the bacterial motility.
During the growth phase, the external flow field together with the interaction between the bacteria and the surface determines the shape of the biofilm. Here we find qualitatively different outcomes

depending on parameter choice. On the other hand, the growing biofilm changes the space available to the fluid. By applying our model to a simple porous structure, we show how flow paths can be altered or even blocked.
The model has potential for simulating the early stages of MICP and is being extended to also include the precipitation process.

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Effect of Fracture on Reactive-Density-Driven Convection of Injected CO2 in Porous Reservoir

Author: Paiman Shafabakhsh[1]

Co-authors: Behzad Ataie-Ashtiani [2]; Craig T. Simmons [2]; Marwan Fahs [3]

[1] *Student*

[2] *Professor*

[3] *Assistance Professor*

Corresponding Authors: behzad.ataieashtiani@flinders.edu.au, fahs@unistra.fr, craig.simmons@flinders.edu.au, paiman.shafabakhsh@student.sharif.edu

Increasing the global temperature of the Earth's surface due to the accumulation of greenhouse gas in the atmosphere is one of the challenges facing humanity. Carbon dioxide (CO2) is the primary greenhouse gas; thus, minimizing CO2 emissions by storing it in geologic formation reservoirs is an effective way to reduce global warming. Understanding the underlying mechanisms of density-driven mixing and geochemical reactions of injected CO2¬ in geological formations is of the main importance. These coupled processes are affected by the nature of the ambient rocks. Heterogeneity has been found to play a major role in controlling the convective dissolution of CO2. Recently, particular attention has been paid to fractured domains that can be found in several geological reservoirs. Yet, existing studies on the influence of fracture on the fate of CO2 neglect the key processes of geochemical reactions. In this work, we aim at addressing this gap. We investigate the effect of fractures on the coupled convective mixing and dissolution processes during CO2 sequestration. Our methodology is based on numerical simulations. We develop a COMSOL for density-driven convection and mineral dissolution. The fractures are considered explicitly via the discrete fracture model. Based on a hypothetical reservoir with synthetic fractures, we explore the effect of fracture properties and topology on the domain's storage capacity at different rates of CO2 mineral dissolution. It is found that, depending on their topology, the fractures can either help the mixing convection and reaction process or play a restrictive role in entering of dissolved CO2 and hindering the plume fingers from growing. For more representative geology, we investigate the convection-dissolution processes of CO2 on a large-scale outcrop of a volcanic basalt rock formation. Our results show that when thin fractures are neglected to reduce model complexity, the predicted amount of trapped CO2 is underestimated. The storage capacity is more sensitive to fractures at low dissolution rates. The findings are useful for the management of CO2 sequestration in fractured domains.

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Effect of the deformation and variability of biosourced reinforcement mats on their permeability

Authors: Tarek Abdul Ghafour[1]; Chiara Balbinot[1]; Nils Audry[2]; Florian Martoïa[1]; Laurent Orgéas[2]; Pierre J.J. Dumont[1]

[1] *Univ. Lyon, INSA-Lyon, CNRS UMR5259, LaMCoS, F-69621 Lyon, France*

[2] *Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000 Grenoble, France*

Corresponding Authors: chiara.balbinot@insa-lyon.fr, florian.martoia@insa-lyon.fr, laurent.orgeas@3sr-grenoble.fr, tarek.abdul-ghafour@insa-lyon.fr, pierre.dumont@insa-lyon.fr

Biosourced fibres such as flax fibres appear as a credible alternative to glass fibres as reinforcement materials in semi-structural composite parts owing to their low density and good specific mechanical properties. They are also particularly interesting because of their damping properties. Biosourced reinforcements can be used to make prepreg materials using compression moulding processes. They can also be preshaped and impregnated by a thermoset resin using various liquid composite moulding processes such as resin transfer moulding (RTM). During the impregnation, the liquid polymer matrix flows through the fibrous preform. Flow phenomena are altered by the variability and the anisotropy of the porous microstructure. A poor control of the impregnation phase lead to the formation of voids and undesirable fibre damages, orientation and spatial distributions, which is detrimental for the quality of the produced composite parts.
In this study, the effect of the transverse compression of dry flax fibre mats on their anisotropic permeability was investigated. This deformation mode was chosen so as to mimic the compaction to which the fibrous reinforcements are subjected during the composite forming processes. For that purpose, flax fibre mats were subjected to compression tests using a micro-press that was installed on a synchrotron x-ray microtomography (ID19 beamline, ESRF, Grenoble, France). This enabled 3D images of the samples at different compression strains to be obtained. Using dedicated image analysis tools, several microstructure descriptors of the pore (porosity profiles, pore size distributions and tortuosity) and solid (fibre orientation, mean intercept length and specific surface area) phases were quantified.
The permeability tensor of the deformed flax fibre mats was estimated from the 3D images using (i) fibre scale CFD simulations based on the homogenisation method with multiple scale asymptotic expansions (Geodict) and (ii) an analytical model. In the latter case, the Kozeny-Carman model was adapted and used to estimate the anisotropic permeability tensor of non-woven fibrous reinforcements from the aforementioned microstructure descriptors. Besides, the effect of the microstructural variability of fibrous reinforcements (e.g., fibre content, fibre slenderness, spatial distribution and orientation of fibres) on the evolution of their permeability properties was numerically assessed. Results highlight the effect of compression on the permeability tensor. In addition, provided a proper estimation of the microstructure descriptors from the 3D images, the predictions of the permeability properties given by the Kozeny-Carman model nicely fit those obtained using fibre scale CFD simulations.

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Role of mineralogy in controlling fracture formation

Authors: Olivia Brunhoeber[1]; Lauren Beckingham[1]

[1] *Auburn University*

Corresponding Authors: leb0071@auburn.edu, omb0005@auburn.edu

Geologic CO2 sequestration is anticipated to play a major role in minimizing the effects of climate change. For these systems to work they need an impermeable caprock layer, e.g. shale, to prevent injected CO2 from escaping the formation. However, caprock fractures pose a risk to leakage of the injected CO2. In the presence of fractures, the injected fluid will interact with whatever minerals are exposed on the fracture walls. This interaction between the fluid and exposed minerals may result in mineral dissolution and precipitation reactions that enhance or reduce fracture permeability. These reactions, however, are not well understood. In this work, we seek to understand what role mineralogy plays in the formation of fractures to more accurately predict what minerals will be exposed and react with the injected fluid. Because precipitation and dissolution reactions subsequently dictate the evolution of fracture aperture and permeability, it is necessary to the integrity of the system to accurately predict these reactions and their time scales. In this work, shale cores from the Mancos and Marcellus formations are fractured by unconfined compression until an initial fracture forms. The unaltered fracture surfaces are imaged using Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS) to quantify the surface mineral distribution. When the fracture surface composition is compared to X-Ray Powder Diffraction (XRD) data of the formation there are significant discrepancies. The Mancos formation is expected to contain 58.6 percent quartz, 2.3 percent kaolinite, and 4.3 percent calcite, for example. However, Mancos shale consists of at least two distinct strata and as a result, so does the fracture surface. The dominating layer at the fracture surface contains 8.3 to 9.2 percent quartz, 68.3 to 78.2 percent kaolinite, and 3.6 to 6.5 percent calcite. The layer less prevalent at the fracture surface contains 25.1 to 40.0 percent quartz, 26.7 to 48.5 percent kaolinite, and 21.9 to 22.3 percent calcite. Despite these different layers, the fracture occurred predominately at kaolinite-kaolinite interfaces. The Marcellus formation is expected to contain 47.9 percent quartz and 27.1 percent calcite. The fracture surface, however, contains about 0.7 percent quartz and about 97 percent calcite, where the fracture occurred predominately at calcite-calcite interfaces. These results suggest that in Marcellus shale the fracture will be much more reactive than expected from the XRD data alone.

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PORE-NETWORK MODELING OF MINERAL DISSOLUTION AND REACTIVE TRANSPORT IN POROUS MEDIA

Authors: Barbara Esteves[1]; Paulo L.C. Lage[2]; Paulo Couto[3]; Anthony Kovscek[4]

[1] *Stanford University / Universidade Federal do Rio de Janeiro*

[2] *Universidade Federal do Rio de Janeiro (UFRJ/COPPE/PEQ)*

[3] *LRAP/UFRJ*

[4] *Stanford University*

Corresponding Authors: kovscek@stanford.edu, paulo@peq.coppe.ufrj.br, pcouto@petroleo.ufrj.br, besteves@stanford.edu

Reactive transport in porous media and mineral dissolution processes are of extreme interest for many subsurface applications, including CO_2 storage, Enhanced Oil Recovery (EOR), and acidizing for stimulation. A pore-network modeling approach is proposed to understand mineral dissolution regimes during single-phase reactive transport. Our approach solves a coupled transport and reaction pore network model that implements a kinetic model with a single heterogeneous chemical reaction describing the dissolution of calcite by hydrochloric acid solutions. The reactive transport problem is described by the acid mass balance equation in control volumes represented by pores (spheres) and throats (cylinders). The network geometry is updated based on the dissolution process happening at the mineral surface. The fluid flow field is also updated due to these new larger

radii of pores and throats. The use of a data analysis tool based on statistical concepts is introduced as a quantitative criterion to classify the different dissolution patterns. Behavior diagrams are constructed based on a range of dimensionless numbers aiming to identify different regimes and their boundaries. Two- and three-dimensional cubic networks with a uniform distribution of pore sizes were used to study the reactive transport problem, and more complex networks derived from real rock samples. A sandstone and a carbonate pore network were also tested. Comparisons to experimental data demonstrate the applicability of pore-network modeling as a tool to explore reactive transport and mineral dissolution processes, as well as to predict changes in porosity and permeability. Specifically, permeability-porosity relationships, and results that present the various dissolution regimes observed at larger scales, based on direct simulations and experimental trials are compared.

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In-situ Capillary Pressure Measurements for Gaining Insight into Foam Flow in Porous Media

Authors: Eric Vavra[1]; Maura Puerto[1]; George Hirasaki[1]; Sibani Lisa Biswal[1]

[1] *Rice University*

Corresponding Authors: biswal@rice.edu, maura@rice.edu, gjh@rice.edu, edv1@rice.edu

Capillary pressure for foam flowing through porous media was first directly measured by Khatib et. al. in 1987. The capillary pressure was reported to increase with gas fraction up to a certain value above which the capillary pressure remained constant and foam texture coarsened. The value of capillary pressure at which this transition occurred was dubbed the limiting capillary pressure, Pc. *After the study by Khatib et. al., very few foam flow experiments have been published in which capillary pressure is directly measured. More data is needed to completely describe the concept of Pc.* Further understanding of this concept will help build more robust and accurate models for predicting the behavior of foam flowing in porous media.

In our work, we measure *in situ* capillary pressures during foam flow experiments in porous media w

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Study on the effect of pore structure in thermal conductivity and permeability of volcanic rocks

Author: Sandra Vega[1]

Co-authors: Jonathan De la Rosa [2]; Irving Reyna-Bustos [3]

[1] *Centro de Geociencias, Universidad Nacional Autónoma de México*

[2] *Instituto Politécnico Nacional*

[3] *Universidad Autónoma de Guerrero, ESCT*

Corresponding Authors: joni_metroid@hotmail.com, geouact@gmail.com, sandravega@geociencias.unam.mx

Volcanic rocks present a great variety of pore structures that are scientifically intriguing. These pore structures can lead further to a better understanding of geothermal reservoirs, volcanic deposits, and their potential behavior as construction material. In this paper, we study seven volcanic rocks (one ignimbrite, two rhyolites, two trachytes, and two andesites) from Los Humeros Volcanic Complex, at the north of the Trans-Mexican Volcanic Belt. Our focus here is to examine how the particular pore structure of the studied volcanic rocks affects permeability and thermal conductivity (TC). For that, we acquired microtomographic images at resolutions of 26, 10 and 3 microns/voxel. The images were filtered and well segmented to obtain the clearest differentiation between pores and grains as possible. As a reference, we compared the porosity and permeability obtained from the images with experimental data. From the image processing and comparison with the reference values, we conclude that the images at 26 microns/voxel give an overall view of the pore structure, but it lacks enough details. Whereas this last resolution might be sufficient to estimate the thermal conductivity, it is inappropriate for the permeability simulations. In fact, we found that the 3 microns/voxel resolution captures the best whole pore structure in these samples.

The TC simulations of the 3D images of 26 microns/voxel were performed at air, water and steam full saturation and temperatures between 24C and 350C. Our preliminary results show that the values obtained for all samples are between the ranges reported in the literature [1.4, 4.1] W/(K*m). The highest TC corresponds to the rhyolites, followed by the trachytes, andesites and ignimbrite. In general, TC at full water/steam saturation tends to decrease with temperature after 100C. The connected oriented pores and fractures have the highest effects on TC, decreasing its values significantly. Future research will be attentive to extent this work at higher resolutions to cover the better-defined pore structures.

The permeability simulations of the 3D images of 3 micron/voxel were performed for water steam. To better characterize the pore structure in these images, we calculated the tortuosity and Euler number of the connected pore space, and made two different pore networks (PNM). Our preliminary results show that the PNM that has less dead-end pores content is closer to the original image pore structure as it estimates closer values of porosity and permeability. It is to note that the original pore structure of all samples presents very irregular, non-uniform and heterogeneous pore space. There is a general trend between permeability and tortuosity, such as the lower the tortuosity the higher the permeability, except for the andesites. On the other hand, no general trend between Euler number and permeability is found. In contrast with the results of the TC, the effect of connected oriented pores and fractures (increasing the permeability) can be only observed in one of the trachytes; while there is not a clear correlation for the other samples. Consequently, further studies are needed to explain better the effect of these pore structures on permeability.

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Improving physics of residual trapping of CO2 in pore-network flow models using direct numerical simulation

Authors: Amir Kohanpur[1]; Albert Valocchi[1]

[1] *University of Illinois at Urbana-Champaign*

Corresponding Authors: valocchi@illinois.edu, kohanpu2@illinois.edu

The physics of two-phase flow of carbon dioxide (CO2) and brine in natural rocks plays an important role in geological storage of CO2 in deep saline reservoirs as a potential technology to reduce emission of greenhouse gases from conventional power plants. Pore-scale modeling is necessary to understand fundamental behavior of CO2-brine flow through the pores and obtain essential flow properties in field-scale simulation where prediction of amount and fate of trapped CO2 is desired. Direct numerical simulation (DNS) methods and pore-network modeling (PNM) are common approaches to study such flow systems in natural rocks because experimental methodologies are difficult to implement, time-consuming, and expensive. Although PNM is more computationally efficient compared with DNS methods due to simplifications of the pore structure and governing flow equations, PNM does not accurately predict the full drainage-imbibition cycle in terms of residual trapped CO2 and characteristic curves of CO2-brine flow. Our quasi-static PNM simulation on a Mt. Simon sandstone sample from a pilot CO2 injection study showed approximately 70% trapped CO2 at the end of imbibition cycle, which is far greater than typical experimental results on sandstones (about 30-40%) reported in the literature. Such discrepancy becomes severe when the contact angle is relatively small and the rock is more heterogeneous, which is the case in the studied Mt. Simon sandstone sample. This error leads to inaccuracy in the resulting relative permeability and capillary curves which are important inputs of field-scale simulators, and thus, it impacts the predicted fate and distribution of the CO2 plume in the reservoir.
Since the residual trapping of CO2 is mainly due to interface movement in pore elements, the source of this issue is in the defined pore-level flow models in PNM, namely, pre-solved equations of flow and local capillary pressure during piston-type displacement, pore-body filling, and snap-off events. These pore-level events have different contributions to the resulting trapped CO2 after a drainage-imbibition cycle. Our preliminary simulations show that snap-off in pore-throats and pore-body filling are the main factors influencing the predicted residual trapped CO2 at the end of imbibition cycle. Although simplifications in the governing equations of flow and using pre-solved equations form the basis of PNM, they can be revised in terms of wettability, pore geometry, and critical local capillary pressure of events to enhance its accuracy and prediction capabilities in specific flow systems such as CO2-brine. We apply DNS via lattice-Boltzmann (LB) simulation on different pore-network configurations which are small collections of connected pore-bodies and pore-throats. Our goal is to investigate and modify drainage and imbibition pore-level flow and local capillary pressure models of quasi-static PNM in CO2-brine system. Our LB code can predict the shape and evolution of interfaces, flow rate and distribution of each phase, and incorporate viscous and capillary forces. These modified models can be incorporated in a PNM solver to be applied on extracted pore-networks from natural rocks thereby resulting in more realistic macroscopic characteristic curves and residual trapping of CO2.

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Pore network modeling from micro-CT X-Ray data, methodology using open source software and digital rock printing.

Author: Aarón Sánchez[1]

Co-authors: Martín A. Díaz-Viera [2]; Mario Eduardo Ramos García [2]; Rosario Pacheco Serrano [2]; Manuel Coronado Gallardo [2]

[1] *UNAM*

[2] *IMP*

Corresponding Authors: ros.pach.ser@gmail.com, mcoronad@gmail.com, aarnsanchz@gmail.com, mdiazv@imp.mx, mramos@imp.mx

This work presents a methodology and case study for pore network modeling from micro-CT X-Ray data of rock samples, to obtain petrophysical properties (permeability, capillary pressures, and relative permeability). The use of open source software for every step of the methodology is highlighted. The methodology can be split in two parts the first is the acquisition of the data, image processing using ImageJ, network extraction (from different authors) and analysis of data from the micro-CT images. The second part is the Pore Network Modeling using OpenPNM, that includes the construction of the model and the petrophysical properties calculations. The methodology is applied to two Bedford sample rocks.
As a further study, the obtained models are altered to achieve a printable scale and be printed on a 3D printer with resin and wax as materials.

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Relaxing the Capillary Equilibrium Constraint for Automated Contact Angle Measurement of Time-Resolved X-ray Micro-Tomography Images in Porous Media

Authors: Omid Shahrokhi[1]; Amir Jahanbakhsh[1]; M. Mercedes Maroto-Valer[2]

[1] *Heriot-Watt University*

[2] *Research Centre for Carbon Solutions (RCCS), School of Engineering and Physical Sciences, Heriot-Watt University, UK*

Corresponding Authors: a.jahanbakhsh@hw.ac.uk, m.maroto-valer@hw.ac.uk, o.shahrokhi@hw.ac.uk

The advances in pore-scale imaging in the past decade have enabled routine imaging of multiphase flow in porous media. This has allowed in-depth studies of governing multiphase flow mechanisms at the pore-scale. However, most of these studies are performed on static images of fluid/fluid interfaces in porous media due to ease of access to smaller X-ray flux sources available in lab-based systems. More recently, high-quality time-resolved data acquired by high flux X-ray synchrotron imaging [1,2] has enabled the micro-scale study of non-equilibrium fluid invasion events that are more directly relevant to fluid dynamics 3. The present work focuses on improving dynamic contact angle measurements by relaxing the capillary equilibrium constraint (constant fluid/fluid interface curvature) required by existing automated contact angle measurement methods [4,5] to infer the actual location of the three-phase contact line.

We present a method for automated contact angle measurements along three-phase (solid/wetting/nonwetting phase) contact lines that can output separate contact lines for each specific ganglia. The method extracts the contact surfaces between phases from segmented images by employing the Delaunay refinement method [6] for surface mesh generation. The method by default respects the boundaries and does not split them with triangle facets, and thus preventing the method from moving the contact lines during surface generation from voxels. This allowed us to relax the constraint of constant curvature of the fluid/fluid interface (at capillary equilibrium) that is required by other available methods to infer the actual location of the three-phase contact line [4,5]. This can potentially allow more accurate measurement of dynamic contact angle measurements or experiments where the time

scale is likely too short to establish full capillary equilibrium [7,8]. Depending on the parameters of the methods (facet size, facet distance and cell size), minimal smoothing could be introduced into the method while maintaining the integrity of observed features (general guidelines are advised based on image resolution of the size of features of interest). Moreover, extra Gaussian smoothing of the solid or fluid/fluid interface or the contact line is not required for this method. The three-phase contact line is defined as the set of vertices common to the surface of all phases. At these vertices, the normal vectors of the solid surface ($\vec{a}$) and the fluid/fluid interface ($\vec{b}$) are calculated. The contact angle (the angle between tangent planes to the solid surface and fluid/fluid interfaces) in each vertex is then calculated from equation 1:

$$\theta = cos^{-1} \frac{\vec{a}.\vec{b}}{|\vec{a}||\vec{b}|} \quad (1)$$

The algorithm is then validated using synthetic images of an idealized geometry (sphere of non-wetting phase) that is intersected at known angles with a solid plane [9]. Furthermore, we employ the method to provide dynamic contact angle distribution for each separate contact lines of selected ganglia in time-resolved synchrotron data [8] and verify the measurements by manual contact angle measurements.

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Inverse Gas Chromatography–a way to determine structural and surface chemical properties of the internal rock surfaces for core-scale wettability characterization

Author: Maja Ruecker[1]

Co-authors: Majid Naderi [2]; Daryl Williams [1]; Apostolos Georgiadis [3]; Paul F Luckham [1]

[1] *Imperial College London*

[2] *Surface Measurement Systems*

[3] *Shell Global Solutions International B.V.*

Corresponding Authors: mnaderi@surfacemeasurementsystems.com, m.rucker15@imperial.ac.uk, d.r.williams@imperial.ac.uk, a.georgiadis@shell.com, p.luckham01@imperial.ac.uk

Wettability, the tendency of a solid medium to stay in contact with one fluid in the presence of another, is a key factor influencing multiphase flow in porous rocks as it occurs for instants during oil production from oil-reservoirs. In addition to the average wettability, which is often described through adhesion forces, surface energies or contact angle measurements, the spatial distribution of wettability in the porous rock can be significant. These variations in substrate wettability may be related to the intrinsic surface chemistry of constituent minerals, and well as surface roughness.
In this work, we assessed the relationship between wettability, mineralogy and surface structure for two rocks: Ketton carbonate, which is effectively chemically homogeneous comprising 99.9% calcite; and Bandera Brown sandstone which contains different minerals such as quartz, kaolinite, plagioclase, calcite and illite. This work utilizied inverse gas chromatography (IGC) and builds on previous studies where micro-computed x-ray tomography and atomic force microscopy were used to assess visually, how the different wettability-controlling parameters influence the core scale response [1,2]. However, one limitation of both micro-computed tomography and atomic force microscopy is the small sample size (typically 10's of ⊠m scale), which can barely be considered representative. IGC, on the other hand, is capable of determining molecular and structural properties of the internal rock surface along the length of a Darcy-scale plug through the determination of surface energies and surface areas using a set of probing gases over say 0.1-0.5 m2 of surface 3. We have investigated the variation in surface energy distributions and surface area for a range of different humidities and found that the chemical and structural characteristics as determined by IGC are sensitive to changes in substrate mineralogy. In the case of the sandstone, a range of surface energies were determined, as a function of enviromental humidities leading to a variation in surface mineralogy exposed to the gaseous phase. Due to capillary condensation, the humidity in the systems can be related to a specific capillary pressure. The new methodology we present allows us to relate the capillary pressure to the surface area and mineralogy when an invading non-wetting fluid is introduced.
IGC provides a full description of the surface energy, chemical and structural attributes of the internal rock surfaces at a representative scale through this relationship provides a key link to upscale molecular attributes, such as wetting or wetting alteration.

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Petrophysical properties predictions using computerized tomographic images

Author: Manuel Ramon Vargas Avila[1]

Co-authors: Adna Grazielly Paz de Vasconcelos [2]; Carlos Eduardo Menezes dos Anjos [1]; Lizianne Carvalho Medeiros [1]; Alexandre Gonçalves Evsukoff [1]; Rodrigo Surmas [3]

[1] *COPPE/UFRJ*

[2] *COPPE/ UFRJ*

[3] *CENPES/PETROBRAS*

Corresponding Authors: adna@coc.ufrj.br, manuelvargas760@gmail.com, surmas@petrobras.com.br, liziannecarvalho@gmail.com, alexandre.evsukoff@coc.ufrj.br, carlos.menezes@poli.ufrj.br

Computed tomography (CT) has been widely used to obtain petrophysical properties, due to its ability to imaging three-dimensional portions of reservoir rocks, allowing, for example, to monitor fluid flow simulation experiments 1 and matrix acidification process 2. Models can also be extracted from the images for simulation and obtaining a series of properties, such as: mechanical properties 3, electrical properties [4], mineralogical composition 5, among others. Since the initial applications [6], advances in acquisition systems have made it possible to obtain better quality images in a short period of time enabling the use of this technology in large scale. As part of the basic petrophysics laboratory process, some regions of the core sample are plugged for the purpose of estimating the petrophysical properties. Using this punctually measures in conjunction with CT core profile images is possible to estimate petrophysical properties on a core scale or even to calibrate well logs, in regions where the well log resolution is not capable to identify certain levels of heterogeneity [7], or when the presence of factors that can hinder the interpretation of profiles, such as invasion of drilling fluid or vugular porosity [8], for example. The previous statements motivate the development of the present work. In recent years, deep learning models have achieved satisfactory results in automatic analysis of images and texts, being the state of the art in many computational vision tasks such as image classification and segmentation [9-11]. Inspired by the previous works we propose the use of deep learning models for estimating petrophysical properties using tomography core images. The model selected consists in a convolutional neural network architecture named as VGG 19 [12], adapted for regression problems restructuring the fully connected layers. The choice of this architecture is due to its success in different problems of computer vision and the existence of pre-trained models in large databases which can be reused using the technique known as transfer learning [13], this is necessary. In this case, we use a pre-trained model in Imagenet dataset [14]. The dataset used for model training consists of 1085 regions of tomography images extracted from 6 wells with their respective porosity value. To evaluate model performance we use a cross validation scheme where in each fold a well is separated for model testing. The results show that it is possible to be successful in predicting porosity in regions that have not been part of the model training. A comparison of the porosity profile predicted by the model and the NMR profile confirms the good performance of the model.

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Lithology classification on rock samples microtomographic images using artificial intelligence

Author: Carlos Eduardo Menezes dos Anjos[1]

Co-authors: Manuel Ramon Vargas Avila [1]; Adna Grazielly Paz de Vasconcelos [1]; Lizianne Carvalho Medeiros [1]; Alexandre Gonçalves Evsukoff [1]; Rodrigo Surmas [2]

[1] *COPPE/UFRJ*

[2] *CENPES/PETROBRAS*

Corresponding Authors: carlos.menezes@poli.ufrj.br, adna@coc.ufrj.br, liziannecarvalho@gmail.com, surmas@petrobras.com.br, alexandre.evsukoff@coc.ufrj.br, manuelvargas760@gmail.com

Three main properties are linked and closely related to reservoir feasibility: porosity, permeability, and also lithology 1. In order to properly characterize pre-salt carbonate reservoirs, it is particularly important to understand the inherent geological peculiarities related to lithology. Accurate discrimination of lithology helps to reduce the error in the prediction of permeability and hydrocarbon volume from well log as well as to understand the depositional and diagenetic processes, which are also closely correlated with implications for fluid flow properties 2. Commonly, two-dimensional thin-section photomicrographs are the kernel of lithology definition 3. However, this procedure could have a certain subjective level depending on the chosen attributes used for the expert 1. In addition, thin-section images are strictly bidimensional and delineate a small area, besides being destructive. In contrast, x-ray computed microtomography has become a standard technique in reservoir characterization workflows [4] because it allows a representative description of three-dimensional microstructure, closely related to thin-sections and straightforward to interpret. Further, artificial intelligence algorithms have been demonstrating excellent performance in tasks such as computer vision. Related to the oil and gas industry, these algorithms achieved useful applications within different data domains, such as seismic data and well log data, for instance. Convolutional neural networks have been successfully applied to recognize grain size distribution 5, estimate P- and S-wave velocities [6], estimate permeability values simulated with pore network approach [7], among others. Therefore, the application of deep learning is proposed for the identification of lithological patterns on microtomographic images of rock samples, to automate lithology classification. Two convolutional neural network models were proposed and implemented: a base model and this same model modified by adding a layer of spatial pyramid pooling (pooling strategy), where both were compared with the use of the transfer learning technique on the model Inception v3. As benchmark for these models, classic methods for extracting characteristics from images were used as input to a multilayer perceptron. The dataset of interest has samples of 60 plugs, which are distributed in three different classes, labeled by specialists. Each plug has 100 images available for use, thus summing up to 6,000 images. The results obtained showed that the Inception v3 model surpassed, on average, the other models, reaching over 80% of average accuracy. With that, further studies are being developed to automate the lithology classification of Brazilian pre-salt carbonate samples by categorizing microtomographic images using deep learning algorithms in a non-destructive way.

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Facilitating the Reproduction of Simulation Results

Authors: Bernd Flemisch[1]; Dennis Gläser[None]; Timo Koch[None]; Martin Schneider[1]; Kilian Weishaupt[1]

[1] *University of Stuttgart*

Corresponding Authors: kilian.weishaupt@iws.uni-stuttgart.de, martin.schneider@iws.uni-stuttgart.de, timo.koch@iws.uni-stuttgart.de, bernd@iws.uni-stuttgart.de, dennis.glaeser@iws.uni-stuttgart.de

Guaranteeing the reproducibility of simulation results faces many technical challenges, mostly originating from complex software stacks and hardware architectures. In this talk, we present our measures for facilitating the reproduction of simulation results obtained with the open-source porous-media simulator Dumux. In particular, we would like to automate the steps from a local executable to a distributable web application with which the results can be reproduced and visualized. This includes the containerization of the underlying software stack, access to the required input data, selection and provision of a suitable backend, as well as the generation of the browser frontend. The current state of our efforts is illustrated by means of a recently performed benchmark study for flow and transport in fractured porous media.

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Assessment of end-effects during two-phase flow in micro-fluidic model pore networks –is it possible?

Authors: Marios Valavanides[1]; Nikolaos Karadimitriou[2]; Holger Steeb[3]

[1] *University of West Attica*

[2] *Institute of Mechanics (CE), Stuttgart University*

[3] *University of Stuttgart*

Corresponding Authors: holger.steeb@mechbau.uni-stuttgart.de, marval@uniwa.gr, nikos.karadimitriou@mechbau.uni-stuttgart.de

Two-phase flow in porous media occupies a central position in physically important processes with practical applications in the energy, environment and chemical industry. Many research efforts are focused on furnishing models that can describe process phenomenology across different domains of size and time scales and for a variety of operating conditions. Yet, upon implementation, they all come across a stumbling-block, the correct compilation,interpretation and integration of regular or special core analysis (R/SCAL) laboratory data into true-to-mechanism constitutive relations, i.e. Darcy-type relative permeability expressions, over representative elementary volumes (REVs) pertaining to the field scale.
The cause of the problem lies on the sudden change of flow conditions, as the test fluids enter the core during R/SCAL. The flow switches from purely viscous within the injection tubing, to simultaneous, mixed viscous/capillary flow within the tortuous pore network of the core. The immiscible, interstitial flow is reorganizing along an entry zone until it adapts to a fully developed pattern 1. Consequently, the measured values of pressure gradients, saturation and flow rates, necessary to evaluate the true constitutive relation at the REV scale, are biased. Similar conditions settle at the exit ports. This phenomenon is commonly described as "*End-Effects*". It may be substantial or not, depending on the physicochemical properties of the NWP/WP/PM system and the flow conditions. End-effects distort the equivalence between the measurements during core flow and true/actual REV flow and that has an impact on the specificity of field scale simulators.
To address the problem, we propose to deploy a systematic laboratory study with two objectives; (a) to validate the specificity of a recently proposed theoretical framework (*DeProF*) [2,3] for two-phase flow within **micro-fluidic model pore networks**, and confirm the existence of latent process characteristics, i.e. the flow rate dependency of relative permeabilities -described by a universal scaling law, the existence and uniqueness of a locus of Critical Flow Conditions (CFCs) and corresponding system-specific **characteristic process invariants** [4,5]; (b) to correlate the structure of the CFC locus and associated invariants with the structure of the interstitial flow patterns. Microfluidic pore networks are ideal for both purposes because of short times to reach steady-state and direct visual observation of the interstitial flow patterns [6].
The underlying idea is to tap on the uniqueness characteristics of the locus of Critical Flow Conditions and characteristic process invariants, inherent in steady-state two-phase flow in pore networks, and their effectiveness in describing the asymmetric effects of capillarity across the entire flow regime. The CFC locus can be used as an effective "phenotype" of the pore network and, as such, it may be possible to use it to identify more efficiently the extent of end-effects during R/SCAL studies. The scope is to be able to evaluate their magnitude during R/SCAL without direct inspection of the interstitial flow structure [7,8,9], but, ideally, just from macroscopic measurements. Upon success, new opportunities will open on reconfiguring existing R/SCAL protocols with smarter ones.

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Experimental Evaluation of the Saturation Vapor Pressure above Supercooled Nanoconfined Liquids

Authors: Klaus Schappert[1]; Rolf Pelster[1]

[1] *Universität des Saarlandes, Experimentalphysik*

Corresponding Authors: rolf.pelster@mx.uni-saarland.de, k.schappert@mx.uni-saarland.de

The saturation vapor pressure p_0 above an adsorbate is a fundamental quantity for the analysis of sorption processes. For example, it is needed to evaluate the pore size distribution of the hosting medium, the Laplace pressure playing a role in sorption-induced deformation as well as changes of chemical potential due to phase transitions. Above the bulk triple point, T_3^{bulk}, it equals the saturation vapor pressure above the bulk liquid. However, at lower temperatures the correct value of $p_0(T)$ is controversial. It cannot be measured directly, because complete sorption isotherms cannot be recorded: the pressure in a sample cell can only be increased up to a value where gas sublimates at the walls. Here, we show how to determine the appropriate saturation vapor pressure above a nanoconfined supercooled liquid by experiment. For this purpose, we have performed sorption measurements with liquid argon in nanoporous Vycor glass below and above the bulk triple point. Using the Kelvin equation we relate the unknown quantity $p_0(T)$ to the pore radius, $r_P(p_0)$, that is independent of temperature. The knowledge of the absolute values for the liquid–vapor surface tension of the supercooled adsorbate, $\gamma_{lv}(T)$, is not required. However, we presuppose that its dependence on the unknown vapor pressure, $\gamma_{lv}(p_0)$, is bulk-like. Our results for argon indicate that the vapor pressure above supercooled nanoconfined argon is similar to that above supercooled bulk argon. We expect that this experimental method can be generalized to other adsorbates and porous materials with low thermal expansion. Thus, it may be used to detect deviations from the extended (extrapolated) vaporization curve of bulk liquids 1.

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Water Dynamics in Nanoporous Confinement: A Quasielastic Neutron Scattering Study

Authors: Aicha Jani[1]; Benedikt MIETNER[None]; Mark Busch[2]; Jacques OLLIVIER[None]; Bernhard Frick[3]; Markus APPEL[None]; Jean-Marc ZANOTTI[None]; Patrick Huber[4]; Michael Fröba[5]; Denis Morineau[6]

[1] *Phd Student*

[2] *Hamburg University of Technology, Ei{\ss}endorfer Stra{\ss}e 42, 21073 Hamburg, Germany*

[3] *Institut Laue-Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France*

[4] *Hamburg University of Technology*

[5] *University of Hamburg*

[6] *CNRS - Institute of Physics of Rennes*

Corresponding Authors: froeba@chemie.uni-hamburg.de, aicha.jani@univ-rennes1.fr, denis.morineau@univ-rennes1.fr, patrick.huber@tuhh.de

Nanoconfined and interfacial liquid water is ubiquitous in Nature and plays a central role in many applications. This explains why the dynamics of liquid water in spatially confined geometry has been extensively studied, especially using mesoporous silica as a model system and quasielastic neutron scattering (QENS) as a probe of the molecular mobility. According to the abundant QENS literature, it appears that the chemical nature of the surface of nanoporous materials can be envisioned as a driving parameter of water dynamics.

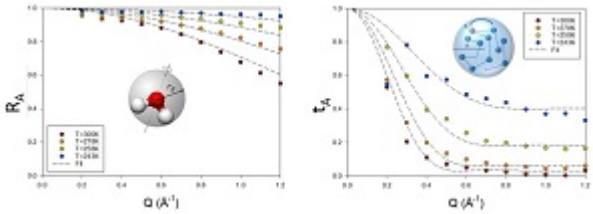

Figure 6: Figure: Relaxation modes related to water dynamics in nanopore. Isotropic molecule rotation (left panel) and confined translational jump diffusion (right panel).

This study aimed at making use of this phenomenon in order to tune the interfacial mobility of nanoconfined water using different surface-water interaction. Periodic silicates and organosilicates were used to investigate the effect of fully hydrophilic or alternating hydrophilic and hydrophobic surface interaction on the dynamical properties of water confined therein. Different temperatures and matrices were used, while keeping the pore size constant. Water translational and rotational dynamics was assessed experimentally by modelling the different relaxation modes composing the incoherent dynamic structure factor (cf. Figure).

ACKNOWLEDGMENTS
Support from Rennes Metropole and Europe (FEDER Fund –CPER PRINT2TAN), and the ANR (ANR-DFG Project NanoLiquids N° ANR-18-CE92-0011-01) is expressly acknowledged.

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Upscaling of a Cahn–Hilliard Navier–Stokes Model with Precipitation in a Thin Strip

Authors: Lars von Wolff[1]; Iuliu Sorin Pop[2]

[1] *University of Stuttgart*

[2] *Hasselt University*

Corresponding Authors: sorin.pop@uhasselt.be, lars.von-wolff@mathematik.uni-stuttgart.de

Multiphase flow and reactive transport are important in many applications, for example in porous media. We consider the incompressible flow of two immiscible fluids in the presence of a solid phase changing due to precipitation and dissolution of ions. On the pore-scale we employ a phase-field model that extends the widespread two-phase models to the ternary case by including a solid phase. To upscale this model to the Darcy scale, we consider it in the geometry of a thin strip. In the context of porous media the thin strip can be seen as the representation of a single pore. For scale separation we introduce β as the ratio between width and length of the strip. Using asymptotic expansions we investigate $\beta \to 0$ under moderate assumptions on Peclet number and Capillary number. The resulting multi-scale model consists of upscaled equations for ion transport and flux, while the phase field equation has to be solved in cell-problems on the pore scale to determine the position of interfaces. Another important asymptotic limit for phase-field models is the sharp interface limit. Here the diffuse interface width ϵ approaches zero and a sharp interface model is recovered. We find asymptotic consistency of upscaling and sharp interface limit, i.e. the two limits commute. Of interest is in particular the sharp interface limit of the upscaled model. It consists only of Darcy-scale equations, as the resulting cell-problems can be solved explicitly. We conclude with numerical results to compare the obtained models.

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On upscaling pore-scale models for two-phase flow with evolving interfaces, Adv. Water Res., 142 (2020), 103646

1269

Efficiency and Accuracy of Micro-Macro Models for Dissolution/Precipitation in Two-Mineral Systems

Authors: Stephan Gärttner[1]; Peter Frolkovic[2]; Peter Knabner[3]; Nadja Ray[4]

[1] *Friedrich-Alexander-Universität Erlangen-Nürnberg*

[2] *Slovak University of Technology*

[3] *University Erlangen-Nürnberg Department Mathematics*

[4] *Friedrich-Alexander Universität Erlangen-Nürnberg*

Corresponding Authors: ray@math.fau.de, gaerttner@math.fau.de, peter.frolkovic@gmail.com, knabner@am.uni-erlangen.de

Porous media naturally exhibit at least two different spatial scales, on which measurements, modeling and simulations are possible. The pore/micro-scale is the fundamental scale, on which flow and reactive transport processes take place whereas the scale of the porous medium is ultimately of practical relevance. However, geochemical behavior cannot be understood considering this larger scale alone and investigations become increasingly difficult if the dynamically evolving pore-scale structure is taken into account.

In this presentation we introduce an efficient numerical scheme for reactive flow and transport problems in evolving heterogeneous porous media. Building upon micro-macro models obtained from detailed pore-scale models via periodic homogenization, our approach comprises flow and transport equations on the macroscopic scale including upscaled microscopic information (specific surface area, porosity, effective diffusion and permeability) calculated from representative unit cells. Conversely, the macroscopic solutes'concentrations alter the underlying microstructure by triggering dissolution or precipitation processes. This strong bidirectional coupling among both scales in combination with the nonlinear interaction between the solutes'species poses several numerical challenges and requires advanced solution techniques. We present a numerical scheme being capable of evaluating such complex settings. As part of our solution strategy the application of level-set methods provides a convenient and flexible tool to represent even intricate underlying pore-geometries. Using the Voronoi Implicit Interface Method, our framework is also able to accurately describe systems with multiple competing mineral phases. More precisely, complex interactions such as covering processes are accounted for, leading to highly anisotropic structural evolutions. In this way, scenarios beyond the applicability of classical laws for macroscopic parameters such as Kozeny-Carman are accessible with our approach.

We demonstrate the predictive power of our algorithm by comparing to a purely microscopic simulation approach in terms of computational effort and accuracy. For this purpose, the dissolution of an array of dolomite grains within a flow-channel setup is investigated.

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Mathematical modeling of the fate and transport of per- and polyfluoroalkyl substances (PFAS) in the vadose zone

Author: Bo Guo[1]

Co-authors: Jicai Zeng [1]; Mark Brusseau [1]

[1] *University of Arizona*

Corresponding Authors: boguo@arizona.edu, brusseau@arizona.edu, jicai@arizona.edu

Per- and polyfluoroalkyl substances (PFAS) are emerging contaminants of critical concern. As surfactants, PFAS tend to accumulate at air-water interfaces and may stay in the vadose zone for long times before contaminating groundwater. Yet not well understood, the extent of retention in the vadose zone has critical implications for risk management and remediation strategies. We present the

first mathematical model that accounts for surfactant-induced flow and solid-phase and air-water interfacial adsorption. We apply the model to simulate PFOS (a PFAS compound of primary concern) transport in the vadose zone at a model fire-training area site impacted by aqueous film-forming foam (AFFF). Air-water interfacial adsorption, amplified by the low water content due to gravity drainage, is shown to have a significant impact. The retardation factors range from 233 to 1355 for the sand and 146 to 792 for the soil used in the present study. The simulations illustrate that it can take several decades or longer for PFOS to reach groundwater. Counterintuitively, the lower water content in the sand—due to stronger drainage and weaker capillary retention—leads to retardation factors greater than that for the soil. Also, most PFOS is adsorbed at air-water interfaces with only 1-2% in the aqueous phase. Our findings imply that 1) fine-texture materials could have lower retardation factors than sand due to higher retained water content, 2) soil PFAS concentrations are likely to be orders of magnitude higher than those in the groundwater beneath source zones. Both implications are supported by recent field observations at hundreds of AFFF-impacted sites.

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Bayesian inference of poroelastic properties from induced seismicity data using an energy-based poromechanics model

Author: Mina Karimi[1]

Co-authors: Elizabeth S Cochran [2]; Mehrdad Massoudi [3]; Matteo Pozzi [1]; Kaushik Dayal [1]

[1] *Department of Civil and Environmental Engineering, Carnegie Mellon University*

[2] *United State Geological Survey*

[3] *National Energy Technology Laboratory*

Corresponding Authors: kaushik.dayal@cmu.edu, minakari@anderw.cmu.edu, mpozzi@cmu.edu, mehrdad.massoudi@netl.doe.gov, ecochran@usgs.gov

Deep water injection related to shale gas extraction is increasingly relevant for the energy sector. Injected fluids in porous deformable elastic media increase pore pressure, reduce normal effective stress, and change the available friction along factures and faults. Consequently, slip can occur, causing seismic events. Understanding this mechanism and identifying the stress field around the injection wellbores play a central role in assessing the seismic hazard. One of the crucial steps is inferring the unknown model parameters (i.e. poroelastic properties) from the noisy data of injection sites. Due to the indirect relation between the uncertain parameters and the empirical observation (i.e. number of earthquakes and stress drop variations in injection sites) and the high dimension of parameters'domain, the inverse problem is computationally expensive. In this work, we develop a nonlinear forward model by formulating a variational continuum framework of multi-component poromechanics to characterize the evolution of stress, pore pressure, and other mechanical quantities. This is coupled to a probabilistic model that we develop to process collected data, to identify the critical points for crack initiation and to estimate the increasing probability of an earthquake. We adopt a Bayesian inference framework to integrate the partial differential equations (PDEs) of the forward mechanical model with models of uncertainty for observation and parameters. Using this approach, we can project approximate hazard assessments by exploring scenario ensembles generated from the posterior knowledge.

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Introducing the concept of Paradise Island for quantifying the role of subsurface porous media in the green transition

Author: Ali Akbar Eftekhari[1]

[1] *Technical University of Denmark*

Corresponding Author: aliak@dtu.dk

Problem statement
The declining resources of non-renewable fossil fuels combined with the environmental impacts of their combustion have increased the societal demand for switching to renewable resources with considerably lower environmental footprints, often called a green transition. There is not a single solution/path to a fossil-fuel-free life but a combination of solutions that need to be studied and optimized.
The knowledge of the subsurface, accumulated over the last century supported by the now-declining interest in the fossil fuel recovery, can play a vital role in the green transition. It is, however, a complex interdisciplinary concept that requires a good overview of several interconnected topics. This work focuses on developing a simple concept for quantifying the role of subsurface porous media in the green transition.
A convenient concept

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Paradise Island (Fig. 1) is an imaginary land with a variable area and population. It is called paradise because its inhabitants have only technical problems to solve. Their current main technical problem is that their production of fossil fuel is declining and the consumption of oil and gas negatively affecting the climate thus they are looking for alternative resources that are both abundant and clean. They also try to clean up the CO2 emission of their fossil fuel in both point sources (e.g., power plants, factories, etc) by carbon capture and storage and in the distributed sources (e.g., cars, aeroplanes, ships, etc) by alternative low-emission fuels (e.g., biogas, bioethanol, power-to-x, etc). For heating, they want to use low-temperature geothermal resources that can also be recharged with solar heaters. They want to use their knowledge of the subsurface from their fossil fuel production time to use the geological formation for the storage of CO2, synthetic fuels, and hot fluids. Each of these solutions can address part of the problem and requires a certain amount of resources (energy and material). This work presents a workflow for quantifying the environmental footprints and technical feasibility of the subsurface fluid and energy storage solution compared to other alternatives. These solutions are compared in terms of their immediacy and effectiveness, and the extent to which they bring the Island closer to a green state.
Significance and results
The main value of this concept is that by changing the population and surface area of the island and several initial conditions including the energy infrastructures such as power plants, coal mines, oil and gas fields, and import and export of energy the island can be converted to a real country or continent. In this work, two countries of Denmark and Poland are investigated. Among the many alternatives that are studied, the results of fully switching from coal to natural gas or partially switching to windmills, and transport and storage of Polish powerplant CO2 to the Northern Lights

project in Norway are presented. For Denmark, a switch from natural gas to biogas or synthetic fuel storage in the subsurface and the storage of summer heat in the shallow subsurface are studied and their advantages and disadvantages are presented.

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Gas-Oil Displacement Mechanisms in Fractured Vuggy Carbonates at Immiscible and Miscible Conditions

Authors: Xiongyu Chen[1]; Kishore Mohanty[2]

[1] *Center for Subsurface Energy & the Environment, University of Texas at Austin*

[2] *The University of Texas at Austin*

Corresponding Authors: mohanty@mail.utexas.edu, xiongyu@utexas.edu

The fracture-matrix permeability contrast and the oil/mixed-wettability make it difficult to recover oil from fractured carbonate reservoirs. One strategy of increasing oil recovery is to decrease the interfacial tension (IFT) between the invading phase and the oil phase. Gas is good candidate since gas-oil IFT is lower than water-oil IFT and diminishes as gas-oil approaches miscibility. However, the pore-scale mechanisms of gas-oil displacement in fractured media are not well understood.
This work created a fractured medium using a 1.1-cm long and 0.5-cm diameter Texas cream limestone core (matrix) surrounded by sandpack (fracture). We injected methane (immiscible) and ethane (miscible at high pressure) into the oil-saturated fractured medium and monitored the evolutions of oil saturation/concentration using calibrated X-ray computed micro-tomography at a resolution of 10 μm. At immiscible condition, matrix oil saturation change was cyclic instead of monotonic decrease because of spontaneous imbibition. At miscible condition, matrix oil saturation monotonically decreased and we measured that the effective ethane diffusivity in fracture and matrix were 5.07×10−5 and 1.70×10−6 cm2/s, respectively. In particular, gravitationally-unstable oil concentration profile persisted in matrix during the entire miscible experiment, which is likely due to the spatial heterogeneity of matrix effective diffusivity. Last, we found that oil recovery in vugs (size: 10-300 μm) differed significantly from the overall matrix since vugs are not self-connected but are interconnected by smaller inter-granular pores (1-6 μm). The new knowledge acquired by this work should be considered in future dual-porosity simulators to better predict large-scale gas-oil displacements in fractured media.

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Capillary flow mediated drop formation in a yarn-based microfluidic system

Author: BHASKARJYOTI SARMA[1]

Co-authors: AMARESH DALAL [2]; DIPANKAR NARAYAN BASU [3]

[1] *PH. D. STUDENT*

[2] *PROFESSOR*

[3] *ASSOCIATE PROFESSOR*

Corresponding Author: bhaskar.sarma25@gmail.com

Drop formation or generation is the backbone of numerous natural as well as industrial processes, which has been studied extensively by researchers and engineers from centuries both experimentally and numerically. For example, drop-on-demand (DoD) systems have been studied in detail in the context of primarily ink-jet printing and other drop deposition processes, which reveal different aspects of drop detachment and the effect of geometry and fluid properties on the same 3. Similarly, the intricate details of droplet evaporation, condensation, and many more necessary processes have been explored with the advent of high-speed imaging techniques 3.
Again, the spontaneous capillary flow (SCF) or "wicking"through the hierarchical porous structures such as plant tissues, paper, yarn, etc., plays a crucial role in many life-saving processes, household as well as industrial activities which includes drying, coating, filtration, etc. to name a few [4]. Emulating the aforementioned technique of pumpless, capillarity driven flows, researchers have engineered numerous paper (mPAD) and thread (mTAD) based lab-on-chip bio-medical devices 5. However, the added benefits of flexibility and simple assembly, post-manufacturing, of the thread-based devices overpowered its paper-based counterparts, further accelerating the studies in the former area in recent years 5.
Although there are countless studies in both the research areas, namely, "wicking"and "droplet generation", however, we fail to find any study involving droplet formation in a yarn type porous network, thereby bridging the gap between the aforementioned areas. The flow-field engendered by the continuous wicking of an experimental fluid in the complex porous network of a yarn, when suddenly comes to a halt, can give rises to a plethora of interesting dynamics of drop formation, which is studied exclusively in the present work with the help of a simple, yet robust, experimental set-up [6]. We unfurl the dynamics of the air-water-yarn three-phase contact line (TPCL) and the shape evolution of a droplet growing in a freely hanging yarn by using a high-speed visualization system and in-house image processing techniques. Interestingly, the entirety of the associated growth dynamics can be deciphered in three distinct regimes namely, i) radial growth, ii) axial growth, and iii) motion, which is rare in other capillary dominated drop formation studies 1. The subtle interplay between the capillary and the gravitational forces further dictates the transition from one regime to another, which can be determined theoretically by the derived exponential scaling laws involving necessary forces. We have been able to derive a mathematical model that relates the final volume of the droplet generated to the critical volume beyond which gravity dominates the other modes in the course of droplet growth. Further, the universal scaling laws, associated with the capillary end-pinching of a droplet from a non-wettable nozzle, are found to control the dynamics of droplet pinch-off even for this critically low Weber number flow (10^{-4} - 10^{-8}). The proposed droplet generation system is expected to find its applicability in yarn-based biomedical devices as well as can act as a model system while developing flexible, porous, wettable nozzles in the future.

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1277

Towards scalable multi-scale open-source solvers for ionic transport and electrochemistry

Authors: Matteo Icardi[1]; Federico Municchi[1]; Robert Barnett[1]

[1] *University of Nottingham*

Corresponding Authors: matteo.icardi@nottingham.ac.uk, federico.municchi@gmail.com

In this work we present a new open-source solver, based on the finite volume library OpenFOAM, for solving the Stokes-Poisson-Nernst-Planck (PNP) equations and multi-domain, or phase, ionic transfer. The PNP system of equations models the transport of ionic species through diffusion, advection and electrostatic forces, at the microscopic scale. Many applications of said model, also involve heterogeneous reaction occuring at the interface between domains, so appropriate conditions are required. From the microscale point of view, when resolving down to the Debye length, different reactive and non-reactive coupling between the neighbouring domains are implemented numerically in interface conditions that couple the two (or more) computational domains, where respective transport equations of each domain, are solver in a segregated manner. Non-linearities are dealt with a Newton's iterative application of the interface conditions.
Since these simulations are computational intensive, due to mesh resolutions required to resolve the boundary layer and the common porous nature of the domains simulated, a mesoscopic approximated model for dilute ionic solutions, where electro-neutrality holds and the boundary layer effects neglected, can be chosen. Alternatively, a fully macroscopic formulation can be used, where an average over a reference porous medium structure is performed, and macroscopic quantities such as effective diffusion coefficients are determined. For example, the case of a two domain (e.g solid and electrolyte) problem could be represented as a single averaged phase, and so giving a more computationally cheaper model. One such method to do this is homogenisation, where we may formulate corrector equations within the electrolyte domain to couple with the diffusion modes in the electrode domain, therefore bypassing the need for an interface condition.
The proposed OpenFOAM solvers can solve these systems of equations at the micro, meso and macro scales. At the micro and meso-scale, the main challenge is the non-linear coupling through interface conditions between the domains. This is achieved by general domain coupling boundary conditions that allows us to solve the system in a segregated approach that can be easily parallelised, although requiring extra internal iterations. At the macro-scale instead, we propose a novel, yet rigorous approach to deal with solid diffusion in arbitrary solid geometries, by a generalised multi-rate transfer model 3.

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1278

A scale-independent framework for whole brain simulation of blood flow in the human brain.

Authors: Erlend Hodneland[1]; Jan Martin Nordbotten[2]

[1] *NORCE Norwegian Research Centre*

[2] *University of Bergen*

Corresponding Authors: jan.nordbotten@math.uib.no, erlend.hodneland@gmail.com

The human brain contains a highly complex vascular system carrying blood across several magnitudes of scale. On the millimeter scale, the network contains larger vessels that are visible and identifiable with modern imaging technology. However, below imaging resolution, the fine scale network is invisible to current MRI and CT technology, and we can only indirectly observe the net effect of transport of exogenous or endogenous tracers. Simulating blood flow while preserving flow across scales poses several challenges for the model. First, the geometry on the macroscale must be correctly identified. Further, net flow in the unresolved microvessels must be well described. A flow model must also deal with multi-scale flow requiring different model assumptions. Finally, the coupling of 1D flow with 3D flow is challenging and must be handled with care.

In the current work we present a comprehensive flow model for simulation of human brain blood flow within a data-driven geometry, which is an extended model presented in 1. The geometry we derive from state-of-the art MR imaging sequences identifying larger vessels and the brain. Flow in the fine scale capillary network is simulated as porous media flow. Coupling of the flow between larger vessels and the capillary tissue is understood as flow in arterioles and venules. We define a 2-compartment model with an arterial and a venous compartment. The perfusion is modeled as the pressure drop between these two compartments. As a general model assumption, we consider pressure driven flow, according to a model

\begin{align}
& (1) \hspace{1cm} q^N = -k^N(p_i - p_j) \newline
& (2) \hspace{1cm}q^T(x) = -k^T (p^D(x) - p_i) \newline
& (3) \hspace{1cm}q^P(x) = -k^P(p_v^D(x) - p_a^D(x)) \newline
& (4) \hspace{1cm}q^D(x) = -k^D \nabla p^D
\end{align}

Equations (1), (3) and (4) are valid for each of the compartments while (3) is the coupling term. The continuity equation $\nabla \cdot q^{(\cdot)}$ ensures mass balance for (1)-(4) with appropriate sink and source terms.

In this talk, we will present the model in detail. Our results include well-posedness of the model formulation both in the continuous and discrete sense, as well as an efficient numerical implementation 2. We apply the model to physically derived parameters on a real data-set of the full human brain. This allows us to reproduce digitally flow fields in the brain, which otherwise are only available indirectly from invasive measures of tracer (bolus) injections.

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Multi-rate mass transfer models and reactive transport in heterogeneous porous media

Authors: Matteo Icardi[1]; Federico Municchi[1]

[1] *University of Nottingham*

Corresponding Author: federico.municchi@gmail.com

Anomalous (non-local in time) transport is a characteristic feature of transport in fractured and heterogeneous porous media 1. Such phenomenon has been described using a number of equivalent formalisms including dual-porosity, integro-differential formulations, time fractional derivatives, continuous time random walk, and multi-rate mass transfer [4]. The latter formalism was first introduced in a semi-empiric fashion 1 and formulated in a rigorous and consistent way only recently as the Generalized Multi-Rate Transfer (GMRT) 2. The main idea behind the GMRT is that the matrix-fracture system can be decomposed in mobile zones (where advection is not negligible) and immobile zones (where advection is negligible), which exchange mass at different frequencies (rates) derived from the spectral properties of the transport equation.

Concerning mobile regions, macroscopic advection-diffusion-reaction equations can be obtained employing homogenisation theory in the limit of fixed (in time) Robin boundary conditions. Physically, this is allowed by the large separation of temporal scales between mobile and immobile regions, such that asymptotic techniques can be exploited in the mobile region 3.

This work describes how macroscopic models for transport in heterogeneous porous media can be obtained employing an unified formalism based on the GMRT and two-scale asymptotics with drift and spectral decomposition. We show that the effective transport and reaction coefficients resulting from this method can be computed from appropriate cell problems or obtained through calibration. Furthermore, we present numerical applications to colloidal particles and randomly generated geological media.

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Multiphase mixture models with phase change and filtration in OpenFOAM®

Authors: Federico Municchi[1]; Matteo Icardi[1]

[1] *University of Nottingham*

Corresponding Authors: matteo.icardi@nottingham.ac.uk, federico.municchi@gmail.com

In this talk, we present a range of coupled multiphysics multiphase Partial Differential Equations (PDE) models both at the pore- and Darcy-scale and their OpenFOAM® open-source implementation. We start by introducing the general theory for solid-fluid and fluid-fluid mixture, focusing on variable-density and (poly-)dispersed flows, revisiting standard approximations and their limitations. For partially miscible fluids, we present the Cahn-Hilliard and the non-conservative Allen-Cahn formulation that naturally allows for phase change. This can be alternatively represented with linear or non-linear phase change kinetics. For dense suspensions specific rheological changes, such as ageing, can also be incorporated via additional PDEs for the mixture viscosity.

These models are coupled with filtration/deposition boundary conditions to describe porous membrane and solid walls that can selectively retain particles and subsequently change their filtration properties.
The open-source OpenFOAM® implementation will be discussed and applications to oil-wax and oil-asphaltene precipitation, particle filtration, water desalination, and CO2 storage will be presented.

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Meter-scale core floods and 3D numerical modelling to study the interplay between immiscible viscous fingering and geological heterogeneity

Author: Samuel Jackson[1]

Co-authors: Mojtaba Seyyedi [1]; Michael Clennell [1]

[1] *CSIRO Energy*

Corresponding Authors: mojtaba.seyyedi@csiro.au, samuel.jackson@csiro.au, ben.clennell@csiro.au

Immiscible viscous fingering can occur at the continuum scale when the shock front mobility ratio between two fluids exceeds unity 1. The growth and wavelength of characteristic fingers are largely

controlled by the capillary number, with capillary forces damping the instabilities in analogy to transverse dispersion in miscible systems 2. While fingering can occur even in homogeneous systems, in reality the presence of geological heterogeneity strongly impacts the initialization and growth of the fingers; often what is interpreted as viscous fingering is in fact flow channelling governed by the heterogeneity itself.

It has been postulated that in consolidated media, moderate interfacial tensions typical of subsurface fluids, i.e. 20 –80 mN/m, will damp the formation of fingers in almost any realistic setting 3. However, new evidence using high-order, dynamic mesh numerical simulations has shown the formation of 3D fingers with realistic viscosity and IFT values; high-accuracy numerics and problem initiation were key to successful modelling [4]. To what extent viscous fingering occurs in real geological settings remains an open question, potentially impacting many subsurface flow processes, in particular CO_2 sequestration. The need for rigorous experimental data in consolidated media is paramount, coupled with mesh-independent, high-accuracy numerical simulations.

In this work, we use novel meter-scale core floods and high-resolution 3D modelling to study the interplay between viscous fingering and geological heterogeneity. We utilise 3D X-Ray CT data obtained at the ARRC, Perth, Australia of nitrogen and brine flow in a 0.1m diameter, 1m length Bentheimer sandstone core in various drainage flow orientations; up-dip flow in a tilted core, gravitationally unstable flow in a vertical core and gravitationally stable downwards flow in a vertical core 5. The 3D distribution of porosity and saturation, and structural heterogeneity in the core are characterised using novel image-based techniques [6].

In all the experiments, complex, transient interface dynamics are observed, suggesting 3D viscous fingers are formed and interact with the imaged structural heterogeneity. We use classic finite-difference based simulations and high-order dynamic mesh simulations to study the finger formation in 3D. Initial findings suggest that structural heterogeneity, emerging as capillary pressure heterogeneity, largely controls the observed fingering pattern, even in cases with the highest viscous-gravity instability. The wavelengths, and number of fingers predicted from the simulations agree with the experiments, and are generally larger than the underling heterogeneity correlation lengths. This suggests that while the heterogeneity acts to initiate the fingers, the viscous instability later controls the growth and evolution of the fingering, which would otherwise be suppressed by the inherent capillarity in the system.

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Quantifying wetted area of sediments during multiphase flow in geological porous media

Authors: Deepshikha Singh[1]; Jyoti Phirani[1]

Co-authors: Shantanu Roy [1]; Harish J. Pant [2]

[1] *Indian Institute of Technology Delhi*

[2] *Bhabha Atomic Research Center, India*

Corresponding Authors: roys@chemical.iitd.ac.in, singh.deepshikha00@gmail.com, jphirani@chemical.iitd.ac.in, hjpant02@gmail.com

Wettability is one of the fundamental properties of the reservoir sediments that govern fluid flow in porous media for many applications, such as groundwater remediation, CO2 sequestration and enhanced oil recovery (EOR). In aquifers and oil reservoirs, wettability has a significant impact on the economics of in-situ remediation of NAPLs and in oil reservoirs the economics of oil production due to its affects on imbibition capillary pressure curve, relative permeability, irreducible oil saturation, and irreducible water saturation leading to varied recoveries in different wetting conditions. Contact angle measurement, Amott Harvey index, and USBM method are used to quantifying wettability. These methods do not account for the heterogeneity of the aquifers or oil reservoirs and are performed on a much smaller scale. Recognizing that more fluid-solid interfacial area will be present for the wetting fluid, in this work, we develop a method to quantify fluid-solid interfacial area at different fluid saturations. We use experiments using two tracers for a fluid, one of which is ideal tracer and another adsorbing tracer. The ideal tracer follows oil or water flow in the reservoir and adsorbing tracer dynamically adsorbs and desorbs on the porous surface. We conduct the experiments at various saturations of the liquid at a given wettability condition. We observe a linear dependence of fluid-solid interfacial area with saturation. In future, different wettability conditions will be used to quantify the fluid-solid interfacial area to relate it to the wettability.

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Method of Moments to Characterize a Reservoir Using a Single Non-Ideal Tracer Test

Authors: Deepshikha Singh[1]; Jyoti Phirani[None]

Co-authors: Shantanu Roy [2]; Harish J. Pant [3]

[1] *IIT Delhi*

[2] *Indian Institute of Technology Delhi*

[3] *Bhabha Atomic Research Center, India*

Corresponding Authors: chz178509@chemical.iitd.ac.in, hjpant02@gmail.com, roys@chemical.iitd.ac.in, jphirani@chemical.iitd.ac.in

Tracer tests are widely used to characterize the reservoirs for residual oil saturation and heterogeneity. In a reservoir due to mineral heterogeneity, a tracer can behaves non-ideally due to the adsorption on the rock surface. Besides, the immobile volume in the reservoir also affects the residence time distribution of the injected tracer that shows a long tail in the effluent concentration profile.

History matching using tracer transport simulations or several tracer tests at different Peclet number are used to fully describe the reservoir rock for adsorption behavior and immobile volume. In this study, we present a method of moments to characterize the reservoir rock using a single tracer test for a non-ideal adsorbing tracer and considering the immobile volume in the reservoir. We calculate the higher-order moments of the tracers to estimate the fluid flow properties inside the reservoir. We use a convection-dispersion model for tracer transport with the closed-closed boundary conditions, as they are more relevant to core-flood experiments. We use residence time density curve's moment matching technique to arrive at a method to determine the four parameters, namely, peclet number, fraction of immobile volume, retardation factor, and mass transfer coefficient. This saves a computational time required for matching historical data. We explain all the possible conditions for the flow parameter estimation. From flow pattern estimation, we observed that the first moment depends only on the retardation factor, which is always greater than unity for the non-ideal tracer. The presence of the stagnant volume and adsorption of tracer affect the variance, skewness, and kurtosis of the residence time density curves. A trend was seen in the higher-order moments, to measure model parameters, the retardation factor, dead pore volume, and mass transfer coefficient. We use numerical experiments for single tracer flow for the porous media to get the residence time density curves for the tracer. We compared the assumed values of parameters: peclet number, fraction of immobile volume, retardation factor, and mass transfer coefficient used in numerical experiments with parameters values from our moment matching method, which gives good match.

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Quantifying uncertainty using Monte Carlo method in methane hydrate reservoir simulations

Authors: Neelam Choudhary[1]; Jyoti Phirani[None]

[1] *Indian Institute of Technology Delhi*

Corresponding Authors: jphirani@chemical.iitd.ac.in, neelamchoudharybaiya@gmail.com

The extraction of methane gas from methane gas hydrate deposits can become an efficient energy resource in place of the existing conventional energy resources. The short term production tests indicate the feasibility of methane production from these deposits. Simulations are used to investigate the long-term production potential from these reservoirs. Deterministic simulations are used, however, the uncertainty in the reservoir geology, initial saturations, temperature and pressure conditions in the reservoir can have significant impact on the predictions. This study aims to quantify uncertainty in simulation predictions for uncertainty in initial reservoir parameters using Monte Carlo method. We use class-2, confined, oceanic reservoirs.

The depressurization method provides satisfactory results when a confined aquifer layer is considered below the hydrate layer. An In-house multicomponent, multiphase, thermal, 3-D finite volume simulator has been considered with three components - water, methane and hydrate in four phases - gas, aqueous, hydrate and ice. It has been validated against several other simulators in the code comparison study conducted by US DOE. Energy and mass balance equations are solved in space and time domain to compute the production of gas in a reservoir.

We consider uncertainty in porosity and initial hydrate saturation given by a Gaussian distribution. We observe that gas production is most sensitive to porosity. The standard deviation peak is obtained during the initial days when the gas production is low, followed by a sudden drop in the standard deviation peak as the gas production increases.

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Extension and Limits of Cryoscopy for Nanoconfined Solutions

Authors: Benjamin Malfait[1]; Alban Pouessel[1]; Aicha Jani[2]; Denis Morineau[3]

[1] *CNRS-University of Rennes 1*

[2] *Phd Student*

[3] *CNRS - Institute of Physics of Rennes*

Corresponding Authors: benjamin.malfait@univ-rennes1.fr, denis.morineau@univ-rennes1.fr, aicha.jani@univ-rennes1.fr

The lowering of the melting point of frozen liquids by the addition of a solute is a fundamental and well-established phenomenon. Its early study by Bernoulli dates back to the eighteenth century. The linear relation between the melting depression and the amount of salts dissolved in water, usually known as the Blagden's law was proposed in 1788. About one century later, this prediction was extended to different systems, including organic and inorganic solvents and solutes. This phenomenon was established as one of the three Raoult's laws, which embrace the overall colligative properties of solutions.

When they are spatially confined at the nanometer scale, many fundamental properties of the liquid states are also modified. Experimental and molecular simulation studies on various types of solvents embedded in nanoporous matrixes have reported large confinement effects on the phase behavior, structure and molecular dynamics. In this context, the significance of cryoscopy as well as the colligative nature of the freezing point depression by addition of solutes must be reconsidered in nanoconfined geometry.

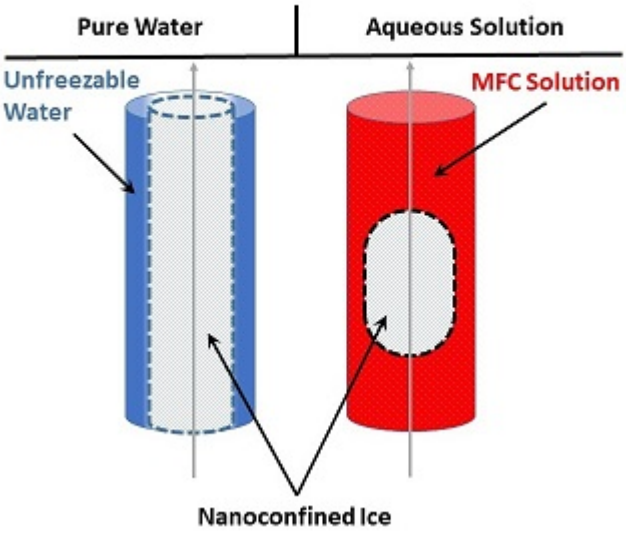

Figure 7: Sketch of the nanoconfined ice for pure water (left) and aqueous solution (right)

This work investigates the phase behavior of aqueous solutions of glycerol confined in MCM-41 and SBA-15 nanoporous matrixes by calorimetry. Limitations due to overfilling and eutectic freezing are prevented by the absence of an external liquid reservoir and by the glassforming property of glycerol. Consequently, the stability of nanoconfined ice in equilibrium with aqueous solutions is studied over a wide range of compositions. In confinement, a large temperature depression of the liquidus line is observed. A thermodynamic model accounting simultaneously for the cryoscopic and the Gibbs-Thomson effects gives a consistent view of the phase diagram for large pores (Rp = 4.15 nm). For smaller pores (Rp = 1.8 nm), it reveals that the water activity strongly deviates from the bulk solution with the same composition, indicating the possible role of concentration heterogeneities in determining the onset of ice freezing in strongly nanoconfined solutions.

This work brings a new insight on a topics founded on two fundamental pillars of the thermodynamics of condensed matter physics (i.e. the Blagden and Raoult's law of cryoscopy and the Gibbs-Thomson effect) and how their combined effects could reveal new phenomena in aqueous solutions confined at the nanoscale.

ACKNOWLEDGMENTS
Support from Rennes Metropole and Europe (FEDER Fund –CPER PRINT2TAN), and the ANR (ANR-DFG Project NanoLiquids N° ANR-18-CE92-0011-01) is expressly acknowledged.

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1286

Pore size distribution in nanoporous materials using NMR cryoporometry

Author: Marc Fleury[1]

[1] *IFP Energies nouvelles*

Corresponding Author: marc.fleury@ifpen.fr

We propose to show the use of NMR cryoporometry for the determination of pore size distribution in the range 2 nm up to 1 µm in nanoporous materials such as natural tight porous media used as diffusive barriers, source rocks saturated with water and oil, and catalysis supports. The principle of cryoporometry is based on the shift of the melting temperature of a fluid when located in a pore [1,2]. A simplified form of the Gibbs-Thomson equation describing this behavior may be written as: ΔT_m (x)=T_m^bulk-T_m (x)=k_GT/x,
where Tmbulk is the bulk melting temperature, x is a dimension related to the pore size and kGT is the so-called Gibbs-Thomson constant. For example, water will melt at -29.1 and -5.8℃ respectively at x=2 and 10 nm (kGT =58.2 K.nm). Using standard NMR equipment, the method is easy to implement for pore sizes below 100 nm. With a different technique to control the temperature initially designed by B. Webber 3 and a low field instrument, the range could be extended to about 1 µm. In addition, we also determine using NMR relaxation measurements the amount of non-frozen fluid at -29℃, yielding the volume below 2 nm. We show different applications of this technique: (i) in preserved shales saturated with their native fluid, we show that the measurements are still valid in the presence of brine (ii) in source rocks saturated with water and oil, we could determine the pore occupancy of water and oil [4] and (iii) in catalysis supports, we could determine the microporosity volume (<2nm) and the pore size distribution of the meso and macro-pores. This results are compared to standard NMR relaxation measurements, nitrogen adsorption and mercury injection data.

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Temperature Distribution (2D and 3D) of Culex Basin-Yellowstone, WY: A comparison of Dirichlet and Neumann nonlinear solutions from field measurements

Authors: Anthony Sorensen II[1]; Peter B. Larson[1]; Sergey Lapin[2]; Jarred Zimmerman[1]

[1] *Washington State University-School of the Environment*

[2] *Washington State University-Department of Mathematics and Statistics*

Corresponding Authors: jarred.zimmerman@wsu.edu, slapin@wsu.edu, anthony.sorensen@wsu.edu, plarson@wsu.edu

Hydrothermal systems are the set of processes that redistribute energy and mass in response to circulating H_2O fluids (Norton, 1984). The Yellowstone hydrothermal system is the surface expression of

the interactions between the Yellowstone hot spot and the overriding North American Plate (Smith et al., 2009). For the past ≈17Ma the record of the Yellowstone hot spot has been recorded in the Yellowstone-Snake River volcanic system, which spans 700km in overall length (Smith et al., 2009). Long-lived areas of concentrated volcanism that take place within the continent, such as the Yellowstone hot spot, are typically associated with plumes of ascending magma (Crough, 1978).

The phase interactions of mass and energy within the Yellowstone hydrothermal system are very complex. It has been established that the phases within the system can ultimately be described by a set of coupled steady-state nonlinear diffusion equation(s) (Faust and Mercer, 1977). With the assumption of a steady-state system, the heat flux at Culex Basin is defined by the matrix conductivity problem where $q(x,y) = -K(x,y) \bigtriangledown u(x,y) = -\mathbf{A} \bigtriangledown u(x,y)$ and is anisotropic with respect to the global Yellowstone hydrothermal system. The diffusive nature of the shallow subsurface layers is defined by White et al., 1971 for a vapor dominated hydrothermal system, such as Yellowstone. The head of the upward heat diffusion within Yellowstone is dependent on the spatial buoyancy $v(x,y)$ with respect to elevation z(m) within the subsurface.

Temperature measurements were taken at ≈68 hot spring locations within Culex Basin. The Levenberg-Marquardt method was used to determine the source term from these measurements. FEniCS/Dolfin libraries were implemented to determine the solution of the variational formulation for the heat distribution at Culex Basin with Dirichlet and Neumann boundaries, respectively (Logg and Wells, 2012). The Dirichlet boundary solution was determined using CG-1 elements in the function space. The local heat flux ($-K(x,y) \bigtriangledown u(x,y)$) and the local heat gradient ($- \bigtriangledown u(x,y)$) were calculated from the results of each solution ($u_D \; and \; u_N$) using P2 elements in vector function space.

Near-surface thermal regimes are highly influenced by active groundwater flow; a useful application of this feature of hydrothermal fields would be to exploit the thermal measurements to obtain velocity/flux fields (Smith and Chapman, 1983). The subsurface distribution of heat in a saturated medium is primarily dependent on the fluid potential and temperature (Smith and Chapman, 1983). Typically horizontal sedimentary layers (i.e. Glacier and rhyolitic ash flows) exhibit hydraulic anisotropy and therefore thermal anisotropy which reduces the advective perturbations to the thermal regime (Smith and Chapman, 1983). The results from the temperature distribution models of Culex Basin will ultimately be used as a component of a multi-phase nonlinear advective-diffusive model for the Yellowstone hydrothermal system.

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1288

The effect of solution gas liberation on oil flow in the porous medium

Authors: Wael Al-Masri[None]; Alexander Shapiro[None]

Corresponding Authors: wafa@kt.dtu.dk, ash@kt.dtu.dk

When the depletion method is applied to produce oil from a volatile oil reservoir, the reservoir pressure starts to decrease, causing the dissolved gas to liberate. The liberated free gas may form disconnected immobile gas bubbles that block individual pore throats, lowering the effective permeability of the reservoir. Unfavorable pore geometry, along with capillary forces/wettability balance, is the main contributor to that possibility.

An experimental study has been designed to determine the mobility of the formed gas bubbles and their effect on reservoir productivity. The experiments involve gas liberation induced by pressure decrease in reservoir rock samples with different permeability and porosity. The pressure is ranging from above to below the saturation pressure, while X-ray computer tomography is applied to detect the in-situ gas liberation. Effective oil permeability versus pressure drop has been monitored as well as the maximum immobile amount of gas (critical gas saturation). In this way, the oil permeabilities under gas saturations below critical have been determined. It has turned out that in low permeable reservoirs formation of the gas bubbles may result in the up to 50% decrease of the relative permeability for oil.

Along with the experimental work, a model for relative permeabilities under two-phase miscible flows in porous media is developed, combining the percolation theory and the methods of statistical physics. It is assumed that gas liberates in the form of the bubbles randomly distributed in a regular capillary network. The corresponding permeability decrease was estimated by the effective medium theory. The model requires four input parameters obtained from the micro-characteristics of the porous medium. Correlations of these parameters with the residual saturations and the exponents in the Corey-Brooks dependences were obtained. A similar model may be applied for gas permeabilities under the condensate precipitation in porous media. It has been demonstrated that the model captures the experimental dependencies available in the literature.

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Capillary bundle-Meter model for non-Newtonian fluid flow in porous media

Author: Takshak Shende[1]

Co-authors: Vahid.J Niasar ; Masoud Babaei [2]

[1] *The University of Manchester*

[2] *University of Manchester*

Corresponding Authors: masoud.babaei@manchester.ac.uk, vahid.niasar@manchester.ac.uk, takshak.shende@postgrad.manchester

The existing empirical shift factor helps to relate steady shear viscosity of a non-Newtonian fluid to the Darcy viscosity in porous media. Depending on the properties of porous media and fluid, the

shift factor varies three orders of magnitude. This makes upscaling of pore-scale steady shear viscosity of non-Newtonian fluids to Darcy scale challenging. To address this issue, we derived Darcy viscosity, effective Darcy shear rate, effective Darcy shear stress, and effective Reynolds number from pore-scale steady shear viscosity using tortuous capillary bundle approach. The proposed capillary bundle-Meter model (CBMM) takes into account S-shaped rheological behaviour of the non-Newtonian fluids (using Meter model), pore-size distribution, and alteration in effective radius due to inherent properties of porous media and non-Newtonian fluid. We validated the proposed model using experimental data from the literature. The proposed model will help simulate non-Newtonian fluid flow at Darcy scale or reservoir scale.

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Recent advances in Mixed Virtual Elements for DFM simulations

Authors: Matias Benedetto[1]; Andrea Borio[2]; Franco Dassi[3]; Alessio Fumagalli[4]; Davide Losapio[4]; Anna Scotti[4]; Stefano Scialò[2]; Giuseppe Vacca[3]

[1] *The University of Queensland*

[2] *Politecnico di Torino*

[3] *Università degli Studi di Milano Bicocca*

[4] *Politecnico di Milano*

Corresponding Authors: anna.scotti@polimi.it, m.benedetto@uq.edu.au, franco.dassi@unimib.it, andrea.borio@polito.it, giuseppe.vacca@unimib.it, stefano.scialo@polito.it, davide.losapio@polimi.it, alessio.fumagalli@polimi.it

The virtual element method is a recently developed numerical scheme for the approximation of partial differential equations on meshes made of polygonal elements with almost arbitrary shape. This peculiarity combined to the robustness of the method to highly distorted and elongated elements makes this technique particularly appealing for the approximation of the flow in fractured porous media, where mesh generation is usually a very complex task, due to the multi-scale nature of the computational domain and to the presence of a large number of intersecting interfaces. The possibility of using polygonal elements greatly simplifies the generation of a mesh conforming to the interfaces, starting from a non conforming mesh. The use of a mixed formulation allows to obtain a locally conservative scheme, suitable for time-dependent transport problems. Here we discuss some recent developments of this methodology and its application to the resolution of the Darcy problem in three dimensional domains crossed by arbitrarily complex networks of fractures.

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Coupling conditions for Stokes-Darcy problems with arbitrary flow directions

Authors: Elissa Eggenweiler[1]; Iryna Rybak[1]

[1] *University of Stuttgart*

Corresponding Authors: rybak@ians.uni-stuttgart.de, elissa.eggenweiler@mathematik.uni-stuttgart.de

Flow and transport processes in coupled free-flow and porous-medium systems have become an active research area over the last decades due to their importance for many environmental and technical applications such as water-gas management in fuel cells, surface-groundwater flows and industrial filtration. Fluid flow in the free-flow region is often described by the Stokes equations, Darcy's law is used in the porous medium and appropriate coupling conditions are applied on the fluid-porous interface. Since the interaction between the porous medium and the free flow is dominated by the interface driven processes, the correct choice of coupling conditions is crucial for accurate mathematical modeling and numerical simulation of flows in coupled systems.

Typically, the conservation of mass, the balance of normal forces and the Beavers-Joseph condition for the tangential velocity are used to couple the Stokes equations to Darcy's law. The Beavers-Joseph interface condition was developed for flows parallel to the porous medium, however, it is often applied for non-parallel flows, even if unsuitable 3. Alternative coupling concepts are either valid for specific (parallel, perpendicular) flows to the interface [2, 5] or contain model parameters which still need to be computed 1. Thus, there is a need for new, more general interface conditions which are valid for arbitrary flow directions and do not include any undetermined parameters.

In this talk, we will present new interface conditions for Stokes-Darcy problems which are valid for arbitrary flows to the interface. These conditions are rigorously derived by means of homogenization and boundary layer theory [4]. All effective coefficients entering the proposed coupling conditions are computed numerically based on the pore geometry, thus, no parameter fitting is needed. The new conditions are validated by comparison of pore-scale resolved to macroscale numerical simulations and are compared to the classical interface conditions. The proposed coupling conditions reduce to the interface conditions derived by Jäger and Mikelić 5, when the same assumptions on flow are made.

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1292

Measuring contact angles in a two-phase flow experiment using home-laboratory micro-computed tomography

Author: Kim Robert Tekseth[1]

Co-author: Dag Werner Breiby [2]

[1] *Norwegian University of Science and Technology*

[2] *Norwegian University of Science and Technology (NTNU) and University of South-Eastern Norway (USN)*

Corresponding Authors: dag.breiby@ntnu.no, kim.r.b.tekseth@ntnu.no

Measuring contact angles with computed tomography using home-laboratory setup is usually limited to static fluid distributions due to the poor time-resolutions that ranges from 30 minutes to several hours per scan. An improved time-resolution on the order of seconds can be obtained with synchrotron sources, allowing contact angle measurements to be conducted during two-phase flow experiments(1). However, synchrotron beamtime is a scarce resource, and it is of considerable interest to develop home-laboratory methods. Here, we demonstrate in situ contact angle measurements during injection of 0.5 M KI doped water into an air-filled 500 μm diameter soda-lime glass bead pack with a flow rate of 0.25 μL/min using a conventional home-laboratory micro-computed tomography setup with a time-resolution approaching 15 s. The good time-resolution has been achieved by combining highly undersampled tomographic datasets with a compressive sensing reconstruction algorithm that exploits a priori sample information(2). With this reconstruction method we were able to geometrically compute contact angles(3) at all timesteps in the 40-minute-long experiment, see Figure 1 for one particular timestep. We believe that the methodology introduced here can make time-resolved computed tomography accessible to the broader scientific community and can further our knowledge about the dynamics of multiphase flow.

1

![Figure 1: A) Segmented cross-section of the reconstructed sample showing the cylindrical container (black), the bead pack (green), the water (blue) and the air (gray) at one timestep. B) Three-dimensional surface-rendering of the liquid (blue), water-air interface (green), and the colored contact line representing contact angle values. The bead pack has been removed for clarity. C) Distribution of contact angles from B) giving a mean value of 72° and a standard deviation of 15°. Scalebar: 500 μm.]

Acknowledgements
We gratefully acknowledge the Research Council of Norway for financial funding through the FRINATEK project 4D-CT, project no. 275182, and the Centre of Excellence funding scheme, project no. 262644 (SFF-PoreLab).

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1293

Dynamic in situ computed tomography study of strain evolution in Draupne shales under triaxial loading

Author: Aldritt Scaria Madathiparambil[1]

Co-authors: Basab Chattopadhyay [2]; Kim Robert Tekseth [1]; Nicolaine Agofack [3]; Pierre Cerasi [4]; Jessica Ann McBeck [5]; Francois Renard [6]; Alain Gibaud [7]; Dag Werner Brieby [8]

[1] *Norwegian University of Science and Technology*

[2] *NTNU*

[3] *SINTEF Industry, Formation Physics Department, PB 4760 Sluppen, 7465 Trondheim, Norway*

[4] *SINTEF*

[5] *Physics of Geological Processes, University of Oslo, Oslo, Norway*

[6] *University of Oslo*

[7] *LUNAM, IMMM, UMR 6283 CNRS, Faculté des Sciences, 72085 Le Mans Cedex 09, France*

[8] *PoreLab, Department of Physics, NTNU, Trondheim, Norway*

Corresponding Authors: dag.breiby@ntnu.no, j.a.mcbeck@geo.uio.no, kim.r.b.tekseth@ntnu.no, francoisrenard99@gmail.com, basab.chattopadhyay@ntnu.no, aldritt.s.madathiparambil@ntnu.no, alain.gibaud@univ-lemans.fr, pierre.cerasi@sintef.no, nicolaine.agofack@sintef.no

Understanding the mechanical behavior of rocks is crucial in current research focusing on extensive storage of CO2 relying on shales as an efficient sealing caprock(1). Current initiatives are now focusing on the evaluation of potential storage in North Sea aquifers. The Draupne Formation forms a several hundred-meter-thick shale layer which acts as a good caprock for deeper reservoirs (2). Computed Tomography (CT) has in recent years evolved as a powerful technique for studying rock mechanics in situ.

1

![Figure 1. Results of in-situ mechanical testing monitored using a core plug of Draupne shale at beamline ID19 at the European Synchrotron Radiation Facility (ESRF). a) Differential stress as a function of axial strain, exhibiting a pseudo-linear "elastic"response. b)-e) Spatial distributions of incremental strain at a differential stress of 32 MPa (red arrow in a), showing b) compaction and d) dilation within the sample. c) The von Mises strain, and e) the maximum principal strain]

Here we present results from experiments performed on Draupne shale using the HADES setup at the ID19 computed tomography beamline of the European synchrotron radiation facility (ESRF), Grenoble (3). We observed an almost linear behavior of the stress-strain during the loading process as shown in Figure (1). Mechanical analysis of the tomography datasets using digital volume correlation (DVC) allowed 3D mapping of the evolving strain tensor fields that provided insights into strain localization accompanying the fracturing process. This study revealed that the pseudo-linear elastic-appearing behavior in the stress-strain plot in fact consists of a series of irreversible processes occurring in the sample. The combination of time-resolved 3D microtomography imaging with 3D DVC analysis (4,5) enabled in-situ investigations of deformation processes via quantification of shear and volumetric strains within the sample, thus providing an improved understanding of the dynamics of the fracturing.

Acknowledgements
We gratefully acknowledge the Norwegian Research Council for funding through Petromaks2 (#280942), FRINATEK (#275182), and the Centre of Excellence funding scheme (#262644).

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1294

Permeability irregularity/hysteresis from micro-channels opening/closing during dissolution/precipitation cycle

Author: Martin Lesueur[None]

Co-authors: Thomas Poulet [1]; Manolis Veveakis [2]

[1] *CSIRO Mineral Resources*

[2] *Duke University*

Corresponding Authors: manolis.veveakis@duke.edu, mlesueur@lbl.gov, thomas.poulet@csiro.au

Permeability is a critical parameter for geological resources characterisation. Its evolution with respect to porosity is particularly interesting and many research initiatives focus on deriving such relationships, to understand some hydraulic impacts of microstructure alteration. Permeability evolution from chemical reactions for instance can become complex as the dissolution of grains contacts or thin wall sections of the skeleton results in the creation of new channels that instantly divert fluid flow and during precipitation, the opposite event of channel closure. In this contribution, we show that this phenomenon can lead to irregular porosity-permeability curves and permeability hysteresis after a dissolution/precipitation cycle. The history-dependent nature of chemical porosity evolution means that static porosity-permeability relationships are not well suited for this kind of modelling and we advocate instead the use of dynamic modelling that takes directly into account the dissolution/precipitation path. We demonstrate our approach by modelling a dissolution/precipitation cycle for a unit cell pore channel and quantify the process at larger scale on three different rock samples, whose microstructures are reconstructed from segmented micro-Computerised Tomography scans. While a micro-channel opening results a localized permeability jump, these discontinuities are smoothed out at the scale of the Representative Elementary Volume but it is the accumulation of those events on the dissolution path that can result in a clear deviation of the permeability from its fitting power law with respect to porosity. The resulting hysteresis after reprecipitation was found to be more pronounced for more channelized and heterogeneous samples and we show that the conventional parameters characterising the microstructure are not the controlling parameters for this permeability hysteresis phenomenon.

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Simulating microscale zero-valent iron injection in field-like conditions: large-scale radial laboratory experiments and numerical modeling

Authors: Federico Mondino[1]; Amelia Piscitello[1]; Carlo Bianco[1]; Andrea Gallo[1]; Tiziana Tosco[1]; Rajandrea Sethi[1]

[1] *Politecnico di Torino*

Corresponding Authors: rajandrea.sethi@polito.it, tiziana.tosco@polito.it, federico.mondino@polito.it, carlo.bianco@polito.it, andrea.gallo@polito.it, amelia.piscitello@polito.it

Using nanoparticles for groundwater remediation –the so-called nanoremediation –is on the way to become a mature technology for the reclamation industry in the next years. This approach foresees the injection of reactive nanomaterials in contaminated aquifer systems, for the direct, fast treatment of contamination hot spots or the contaminated plume. Nanoscale zero-valent iron (nZVI) 1 is today the most material, but also bi-metallic particles 2 and carbon based materials have been proposed [3-5]. nZVI, thanks to its extremely high specific surface area, exhibits a very high reactivity toward a broad set of contaminants, but for the same reason is prone to significant consumption due to side reactions. As an alternative, microscale iron particles (mZVI) have been proposed: they show lower reactivity but longer lifetime, easier and safer handling, and lower commercial costs, thus representing a valid alternative to nZVI with significant advantages in many field applications.
Micro or nanoparticles are typically injected as concentrated slurries either via high-pressure injection using direct push equipment (controlled fracturing approach) or via low-pressure injection through a screened well (permeation approach). A successful delivery (and therefore a successful remediation) depends on the achievement of an effective particle distribution in the target contaminated zone, thus, when technically doable, permeation injection is preferred. In this case, particle transport in porous media is controlled by flow velocity, colloidal stability and the rheological properties of the carrier fluid. As a general rule, mZVI and nZVI dispersed in pure water exhibit poor colloidal stability, resulting in particle aggregation and/or sedimentation, and consequently in an unsatisfying permeation injection. Other particles, eg. iron oxides and graphene oxides [6, 7], are more stable, even though for almost all nano-and micro-materials a kind of colloidal stabilization is needed. Green polymers (guar gum, xanthan gum, starch$\cdots$) are employed to this aim, dosed at few g/L to coat the particles and increase the slurry viscosity, thus preventing aggregation and/or sedimentation for at least a few hours (the time needed for field injection).
In this study, a shear-thinning gel, composed of a guar gum - xanthan gum mixture, was used as particle stabilizer. The slurry rheology and particle mobility in the porous medium were characterized by column transport tests. Then, a radial transport experiment was performed to mimic the particle delivery in more realistic conditions. The gel, even at a low polymeric content (1.75 g/L), proved effective in enhancing the mobility of high concentrated mZVI suspensions (20 g/L) in field-like conditions. A radius of influence of approximately 80 cm and a fairly homogeneous iron distribution were achieved by maintaining a permeation flow. Based only on the information derived from column tests, the MNMs 2018 software (Micro- and Nanoparticle transport, filtration and clogging Model-Suite) was able to predict the particle distribution and pressure build up measured in the radial domain. Experimental and simulated results showed good agreement, thus proving that a simplified experimental-modelling procedure based on 1D column tests can be used to effectively upscale the slurry behaviour to more representative scales e.g. radial domains.

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1296

Unfitted boundary method to improve mesh convergence of high-resolution CT-scan permeability

Author: Martin Lesueur[None]

Co-authors: Hadrien Rattez [1]; Oriol Colomés [1]

[1] *Duke University*

Corresponding Authors: oriol.colomes@duke.edu, mlesueur@lbl.gov, hadrien.rattez@duke.edu

Flow simulations on porous media, reconstructed from Micro-Computerised Tomography (µCT)-scans, is becoming a common tool to compute the permeability of rocks. In order for the value of this homogenised hydraulic property to be representative of the rock at a continuum scale, the sample considered needs to be at least as large as the Representative Elementary Volume. Moreover, the numerical discretisation of the digital rock needs to be fine enough to reach numerical convergence. In the particular case of Finite Elements (FE), the study of Guibert et al. (2015) showed that a mesh size of even twice the resolution of the original image could not be enough to reach mesh convergence for permeability. These two conditions and the increased resolution of µCT-scans to observe finer details of the microstructure, can lead to extremely computationally expensive numerical simulations. While many solutions to the computational limit existing for high resolution CT-scans are developed with the objective to increase the number of elements in a simulation at a lower computational cost, we opt for a different approach which aims at reducing the number of elements needed to reach mesh convergence. To do so, we couple a FE numerical model for Stokes flow in porous media with an unfitted boundary method, which allows to improve results precision for coarse meshes. Indeed, this method enables to obtain a definition of the pore-grain interface as precise as for a conformal mesh, without a computationally expensive and complex mesh generation for µCT-scans of rocks. We demonstrate the advantage of the method on a benchmark of the analytical solution for the permeability of a 3D Poiseuille tube an optimal error convergence rate, quadratic, is obtained compared to the linear obtained with the regular meshing technique. Its performance is validated on three different rock samples, a sandpack, a sandstone and a limestone. We observe a clear improvement of the mesh convergence for the permeability value using the unfitted boundary method. An accurate permeability value is obtained for a mesh coarser than the initial image resolution. The method is then applied to a large sample of a high resolution µCT-scan to showcase its potential.

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A multi-scale nonlinear finite element modelling of subsurface energy storage under cyclic loading

Author: Kishan Ramesh Kumar[1]

Co-author: Hadi Hajibeygi [1]

[1] *TU Delft*

Corresponding Authors: k.rameshkumar-2@tudelft.nl, h.hajibeygi@tudelft.nl

Subsurface geological formations play a crucial role in transitioning towards a greener world. They provide giant capacities for large-scale (TWh) storage of green energy, once this energy is converted to green gas (e.g. hydrogen). The key aspects of successful development of this technology include estimation of safety and storage capacity for a given formation. Formations are often highly heterogeneous, with complex transport and material physics. In this work, we present a computational framework for cyclic loading of rock specimens to estimate the deformation occurring due to non-linear creep deformation. Classical creep and relaxation creep are the two methodologies which are modeled to understand the variation of total strain in the specimen over time. Algebraic multi-scale FE formulation is implemented to reduce the computational cost and accordingly approximate the solution at a fine scale. This study indicates that the algebraic MSFE simulation provides similar results as fine-scale in uni-axial compression.

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How does microbial calcite precipitation alter soil water retention characteristics?

Authors: Ehsan Nikooee[1]; Rahim Saffari[1]; Ghassem Habibagahi[1]; Martinus van Genuchten[2]

[1] *Shiraz University*

[2] *Federal University of Rio de Janeiro*

Corresponding Authors: ehsan_nikooee@yahoo.com, rvangenuchten@hotmail.com, habibg@shirazu.ac.ir, rhm.saffari@gmail.com

In a rapidly changing environment where the extreme climatic events bring about extreme and heavy rainfall events together with extended drought periods throughout the year, new engineering challenges have emerged.

One one hand, the hydraulic and mechanical behavior of top soil layers, in vadose zone, which in such cases experience drastic changes in the degree of saturation would need special attention in engineering projects. On the other hand, new soil stabilization techniques, in which natural soil ingredients (such as soil microorganisms) have been substituted for common chemical additives with high CO2 footprint, have demanded new insights on the hydro-mechanical behavior of such biologically treated soils.

The soil water retention curve (SWRC) is a fundamental characteristic of unsaturated soils which plays an essential role in the soil hydro-mechanical behavior. In order to be able to design treatment scenarios, and predict the soil hydro-mechanical behavior for the partially saturated soils treated biologically, one has to have insights on the alterations induced in SWRC by the biological soil

stabilization technique. There are various soil biological stabilization techniques (e.g., bio-polymer treatment, Microbially-Induced Calcite Precipitation (MICP), and Enzyme-Induced Calcite Precipitation (EICP), ...). In this lecture, our recent studies of the effect of microbial calcite precipitation on the soil water retention curves of coarse-grained as well as fine-grained soils will be presented. The possible contributing mechanisms are highlighted and discussed and future perspectives are envisioned.

Keywords: Soil water retention curve (SWRC), matric suction, microbially-induced calcite precipitation, Bacillus sphaericus, filter paper, pore fluid pH, X-ray diffraction (XRD), micro-fabric, bio-clogging, bio-cementation, soil double layer

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1299

Insights on transition from capillary toward viscous flow in porous media

Author: Mahdi Maansouri-Boroujeni[1]

Co-authors: Mohamed Azaroual [2]; Sophie Roman [1]

[1] *Univ. Orléans, CNRS, BRGM, ISTO, UMR 7327, F-45071, Orléans, France.*

[2] *BRGM, 3 Avenue Claude Guillemin, 45100 Orl´eans, France*

Corresponding Authors: sophie.roman@univ-orleans.fr, mahdi.mansouri-boroujeni@cnrs-orleans.fr, m.azaroual@brgm.fr

Drainage of native fluid in porous media is an intrinsic part of important operations such as CO2 storage and hydrology. The efficiency of these processes depends on the efficiency of the displacement. Front instabilities, known as fingerings, reduce the efficiency of the displacement by leaving some fluid behind. The efficiency of drainage processes depends on invasion pattern and porous media properties, e.g. wettability, etc. Considering the importance of these properties, certain flow regimes based on two dimensionless numbers M (viscosity ratio, $M = \frac{\mu_{nw}}{\mu_w}$, where μ_w and μ_{nw} are respectively viscosity of the wetting and non-wetting phases) and Ca (capillary number, $Ca = \frac{\mu_w \nu_w}{\sigma \sin\theta}$, where μ_w, ν_w, σ and θ are viscosity and velocity of wetting phase, interfacial tension and contact angle respectively) are defined, Fig:1.
Due to the important role of fundamental forces, such as capillary forces, which are not considered in large-scale equations, e.g. two-phase Darcy equation, and undeniable effect that pore-scale mechanisms have on large scale behaviors, the flow should be studied at small scales
In this research, we try to shed light on the mechanisms involved in transition of capillary flow regime toward viscous flow at pore-scale.

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Materials and methods

Microfluidics devices provide us with the well control on the porous media network and pore and throat structure in combination with the transparency and ability of visualization of the phases and the interface by using a high-resolution camera coupled with a microscope. Our patterns were based on the study of Moebius and Or (2012) where they used sinusoidal double capillaries. Water and air were the wetting and the non-wetting phases, respectively, in our PDMS (a silicone elastomer) micromodels to replicate similar situation of CO2 and brine.

Results

Movement of interface in our two sinusoidal channels, with pore-throat size of 160-80μm, varied by manipulation of flow rate. It was observed that, depending on the ratio of viscous and capillary forces, non-wetting phase drained the channels in different manner. The more the viscous forces are dominant in our system, the more involved both channels are, with almost same properties. For lower Ca, however, capillary forces are responsible of the fluid path and position of interface in the structures.

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This preference in flow paths, results in different residual saturation of resident fluid. The system tends to decrease residual saturation by increasing the $\log Ca = -4$ and left behind a portion of fluid in lower -5.25.
It was observed that flow happens as a series of jumps known as Haines jumps. The velocity of these jumps depends on Ca which is in direct relationship with front behavior, so these jumps might be the key parameter for front behaviors. The velocity of these jumps exceeds the average flow rate velocity.

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1300

Component transport at the soil –atmosphere interface

Authors: Insa Neuweiler[1]; Lisa Bahlmann[1]

[1] *Leibniz University Hannover*

Corresponding Authors: bahlmann@hydromech.uni-hannover.de, neuweiler@hydromech.uni-hannover.de

Transport processes in soils are strongly influenced by the time-dependent and complex flow processes at the soil surface. Transport of components in the liquid phase is influenced by the tran-

sient flow conditions driven by infiltration and evapotranspiration. Transport of components in the gas phase is also influenced by the wind field above the soil surface. Component transport at and across the soil –atmosphere interface was and is a topic of several joint research projects with Rainer Helmig, which led to a fruitful and very enjoyable collaboration. A short overview over the topic and the main results of this collaboration will be summarized at the beginning of the presentation.
The main part will focus on the recent studies on gas component transport from soil into the atmosphere. In general, component transport in the gas phase is considered to be mainly due to diffusion. However, the wind field above the soil surface can induce flow into the subsurface and influence transport and mass fluxes. This was studied in laboratory experiments in a sand tank. Dry conditions and partly saturated conditions were considered. Transport under steady state as well as transient conditions was analysed by monitoring gas concentrations inside of the tank. These observations indicate that although transport is mainly diffusive, wind induced lateral transport causes non-symmetric concentration profiles, which in turn influences the diffusive mass fluxes. This effect depends on wind velocities and on the liquid water saturation inside of the porous medium.
The experiments were compared to results of a coupled porous medium flow –free flow and transport model implemented into the environment DuMux. These results demonstrate that it is crucial to consider the coupled problem in order to capture the mass fluxes well. The model results demonstrate that, although the largest difference of the mass fluxes between the different gases is due to the different diffusion coefficients, density effects influence the wind induced lateral flow fields in the porous medium and thus the concentration profiles and related mass fluxes.

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Physical origin of pressure-saturation curves during drainage: modelling based on gravitational and capillary effects, and recipe for upscaling by correcting finite-size effects

Authors: Renaud Toussaint[1]; Monem Ayaz[2]; Gerhard Schäfer[3]; Marcel Moura[4]; Knut Jorgen Maloy[4]

[1] *IPGS, CNRS, Univ. Strasbourg & PoreLab, Univ. Oslo*

[2] *IPGS and LHYGES, University of Strasbourg and PoreLab, University of Oslo*

[3] *LHyGeS, CNRS, University of Strasbourg, France*

[4] *PoreLab*

Corresponding Authors: schafer@unistra.fr, k.j.maloy@fys.uio.no, marcel.moura@fys.uio.no, renaud.toussaint@unistra.fr

We experimentally and numerically study the influence of gravity and finite-size effects on the pressure-saturation relationship in a given porous medium during slow drainage. The effect of gravity is systematically varied by tilting the system relative to the horizontal configuration. The use of a quasi two-dimensional porous media allows for direct spatial monitoring of the saturation. Exploiting the fractal nature of the invasion structure we obtain a relationship between the final saturation and the Bond number $S_{nw}^F = Bo^{0.097}$ using percolation theory. Moreover the saturation, pressure and Bond number are functionally related, allowing for pressure-saturation curves to collapse onto a single master curve, parameterized by the Representative Elementary Volume size and by the Bond and Capillary Numbers. This was done earier without gravity by Moura et al. 2015, and is here extended to any Bond number. This allows to upscale the pressure-saturation curves measured in a laboratory to large representative elementary volumes used in reservoir simulations. The large-scale behavior of these curves follow a simple relationship, depending on Bond and Capillary number, and on the flow direction. The size distribution of trapped defending fluid clusters is also shown to contain information on past fluid flow, and can be used as a marker of past flow speed and direction.

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1302

Dynamic Heterogeneities in Liquid Mixtures Confined in Nanopores

Authors: Aicha Jani[1]; Ramona Mhanna[None]; Benedikt MIETNER[None]; Mark Busch[2]; Jean-Marc ZANOTTI[None]; Bernhard Frick[3]; aziz ghoufi[4]; Patrick Huber[5]; Michael Fröba[6]; Denis Morineau[7]

[1] *Phd Student*

[2] *Hamburg University of Technology, Ei{\ss}endorfer Stra{\ss}e 42, 21073 Hamburg, Germany*

[3] *Institut Laue-Langevin, 71 Avenue des Martyrs, 38000 Grenoble, France*

[4] *university rennes1*

[5] *Hamburg University of Technology*

[6] *University of Hamburg*

[7] *CNRS - Institute of Physics of Rennes*

Corresponding Authors: denis.morineau@univ-rennes1.fr, froeba@chemie.uni-hamburg.de, aziz.ghoufi@univ-rennes1.fr, patrick.huber@tuhh.de, aicha.jani@univ-rennes1.fr

Binary liquid mixtures can exhibit nanosegregation, albeit being fully miscible and homogeneous at the macroscopic scale. This tendency can be amplified by geometrical nanoconfinement, leading to remarkable properties. This work investigated the molecular dynamics of tert-butanol (TBA)–toluene (TOL) mixtures confined in nanochannels by quasielastic neutron scattering and molecular dynamics simulation. It revealed a decoupling of the molecular motion of each constituent of the binary liquid, which can be followed independently by selective isotopic H/D labeling. We argue that this behavior is the signature of spatially segregated dynamic heterogeneities, which are due to the recently established core–shell nanophase separation induced by mesoporous confinement.

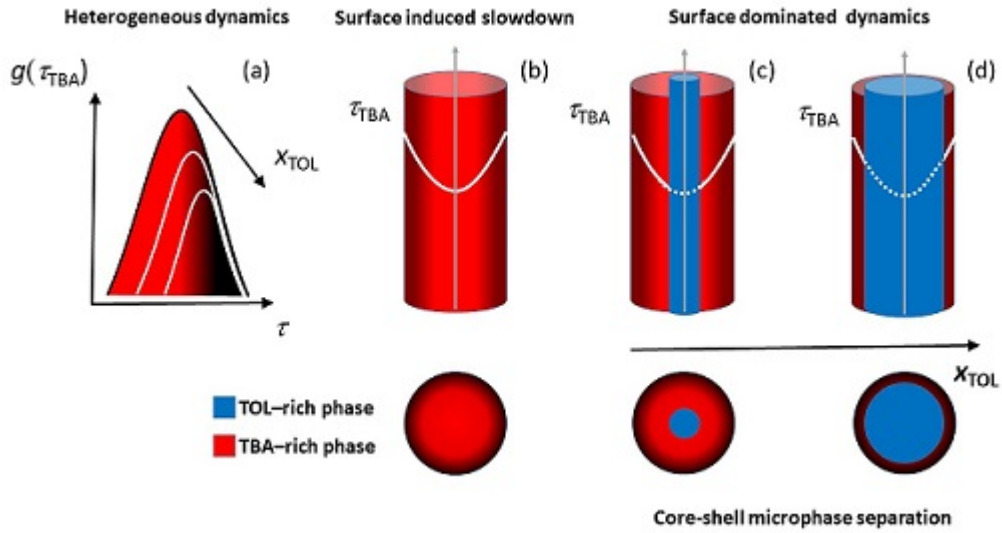

Figure 8: sketch of the core-shell structure

Based on these pioneering studies realized on mesoporous pure silicates (MCM-41 and SBA-15), we have recently extended this work to periodic mesoporous organosilicates (PMOs). We will also discuss the perspectives offered by changing the nature of the organic bridging unit in order to tune the nature of the dynamical heterogeneities of the binary liquids confined therein.

ACKNOWLEDGMENTS
Support from Rennes Metropole and Europe (FEDER Fund –CPER PRINT2TAN), and the ANR (ANR-DFG Project NanoLiquids N° ANR-18-CE92-0011-01) is expressly acknowledged.

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1303

The coupling between compaction and pressurization in cyclically sheared drained granular layers: implications for soil liquefaction

Authors: Shahar Ben Zeev[1]; Renaud Toussaint[2]; Liran Goren[3]; Stanislav Parez[4]; Einat Aharonov[5]

[1] *Institute of Earth Science, Hebrew University of Jerusalem and IPGS, University of Strasbourg*

[2] *IPGS, CNRS, Univ. Strasbourg & PoreLab, Univ. Oslo*

[3] *Geological & Environmental Science, Ben-Gurion University of the Negev, Israel*

[4] *Institute of Chemical Process Fundamentals of the CAS, Prague, Czech Republic*

[5] *Institute of Earth Science, Hebrew University of Jerusalem, Israel*

Corresponding Authors: einatah@mail.huji.ac.il, stanislav.parez@gmail.com, shahar.benzeev@mail.huji.ac.il, gorenl@bgu.ac.il, renaud.toussaint@unistra.fr

The dynamics of saturated granular layers during shaking is controlled by the coupling between grains and fluid. Understanding such systems is crucial for studies of soil liquefaction, seismically induced landslides and shear along faults. This study focuses on the compaction of a near surface well-drained saturated granular layer during seismic shaking. Compaction is known to promote soil liquefaction, but the exact feedback mechanism between compaction and pressurization remains poorly understood. We use Discrete Element numerical simulations composed of coupled solid grains and fluid phases under cyclic horizontal shear of the bottom undrained boundary and a free, completely drained, top layer. We compare the dynamics under two drainage conditions: First, simulations of "infinite"drainage, where the fluid pressure is maintained hydrostatic during the shaking, similar to the model of Clément et al. (2018). Second, simulations of "realistic"drainage in a high permeability layer, whereby fluid pressure dynamically deviates from hydrostatic values due to local granular compaction and dilatation, presented in details by Ben Zeev et al. (2020). Simulation results show two end member behaviors, with a transition controlled by the magnitude of shaking acceleration: At low acceleration the system behaves rigidly, compaction is negligible and fluid pressure remains constant even during "realistic"drainage simulations, where it is allowed to evolve. At high acceleration, significant compaction occurs in both cases, but the compaction rate is higher in "realistic"drainage simulations. This rapid compaction trend is temporally correlated to a transient pore pressure increase that reaches lithostatic stress values before it drops back to a lower value. This is an evidence to a feedback mechanism in which compaction causes pressure increase that can persist under drained condition as long as the compaction rate is sufficiently high. On the other hand, this very pressure itself promotes the high compaction rate. From this we conclude that although well-drained soils are considered liquefaction-resistant, dynamic coupling between pore fluid pressure elevation and compaction during seismic shaking provides a previously unrecognized pathway to liquefaction.

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1304

Chemical Component Transport in Heterogeneous Porous Medium during Low Salinity Water Flooding

Authors: Hasan Al-Ibadi[1]; Karl D. Stephen [2]; Eric Mackay [2]

[1] *Heriot Watt University*

[2] *Heriot Watt University*

Corresponding Authors: k.d.stephen@hw.ac.uk, hha2@hw.ac.uk, e.j.mackay@hw.ac.uk

We investigate the effect that reservoir heterogeneity had on field scale flow behaviour of active ions during Low Salinity Water Flooding (LSWF). We considered that the active ions in LSWF can be salinity or cations. We calibrated behaviour as a function of the degree of variation and correlation length of permeability models. We also examined the effect of fluid mobility.
We modelled LSWF in which wettability is altered due to the reduction of salinity or cation concentration in injected water compared to the formation water. We considered 2D reservoir scale models

to study the impact of crossflow and fingering induced by geological heterogeneity. We compared the salinity profile against the theoretical semi-analytical solution of active ion transport that we developed previously for 1D models (Al-Ibadi et al, 2019). Variations in the complexity of the geological structure were examined via various geological realisations, where the permeability was controlled spatially and randomly distributed for various correlation lengths. This was examined for displacement under various fluid mobilities. The degree of heterogeneity was controlled using the coefficient of variation (Cv), while variogram range was used to control correlation length (Rv). For more details about the model set up, the reader is invited to read Al-Ibadi et al., (2020). This study considered low, medium and high heterogeneity models. We investigated three aspects of the chemical component transport which were: (a) the dispersion coefficient, (b) the mean velocity as defined by advection velocity, and (c) the "Sigmoid-shaped" of the active ion front that is suggested by the complementary error function of the analytical solution.
We found that for very short variogram lengths (i.e. Rv ≤0.015 of the total length of the model) and high coefficient of variation (i.e. Cv≥0.5), an acceleration effect of the salinity front was observed because the heterogeneity induced mixing of the injected and formation water. However, for models with relatively low coefficient of variation, i.e. Cv≤0.5, and short Rv, the heterogeneity mainly affected the dispersion coefficient. For longer variogram length (Rv≥0.14), a deformed chemical component profile was observed, so that the Sigmoid-shaped was no longer preserved, especially for models where the mobility ratio across the low salinity waterfront (the second waterfront) was greater than 1. The resulting profile of the component was deformed by heterogeneity induced fingering on the two phases (i.e. oil and water) additional to the mix that occurs between injected and formation water.
The study provides systematic analysis of the chemical component transport in heterogenous models which is essential to evaluate the performance of LSWF in realistic heterogenous models. The study can be used to enhance the representation of the chemical component in coarse scale reservoir models to capture properly the effect of fine scale behaviour.

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1305

Reducing herbicide spreading in the environment using an eco-compatible nano-formulation

Authors: Monica Granetto[1]; Lucia Re[2]; Carlo Bianco[2]; Aurora Audino[2]; Luca Serpella[2]; Francesco Vidotto[3]; Silvia Fogliatto[3]; Tiziana Tosco[2]

[1] *Politecinco di Torino*

[2] *Politecnico di Torino*

[3] *Università degli Studi di Torino*

Corresponding Authors: carlo.bianco@polito.it, luca.serpella@polito.it, francesco.vidotto@unito.it, monica.granetto@polito.it, silvia.fogliatto@unito.it, lucia.re@polito.it, tiziana.tosco@polito.it

The use of pesticides in agriculture has numerous advantages but also significant environmental drawbacks; The uncontrolled or excessive use of agrochemicals has progressively contributed to the contamination of environmental matrices, and in particular of soils and groundwater. To contribute solving these issues, an eco-compatible nano-formulation was recently developed by the authors to help controlling the environmental dispersion of dicamba, a herbicide widely used to control

broadleaf weeds; dicamba is highly soluble and moderately volatile, but is less toxic and persistent compared to other competing herbicides. The proposed nano-formulation was developed using eco-compatible, low-cost materials, including mineral nanoparticles and food-grade biopolymers, with the aim to reduce dicamba volatilization (thus reducing dispersion in air, and consequently potential impacts on both workers and neighboring crops) and solubility (thus reducing infiltration during and after application, and consequently uncontrolled dispersion in the subsoil).
In this work, the results of laboratory and greenhouse tests are discussed, comparing the efficacy of the nano-formulation against the pure herbicide compound and a commercial dicamba-based product; the efficacy of the nano-formulation was tested in terms of volatilization, mobility in porous media (both saturated and unsaturated) and efficacy in weed control.
Volatilization tests were performed assessing the losses of dicamba over 24 hours from pesticide solutions and soil treated with the different products. Losses from the solutions ranged between 47% for the pure dicamba solution to less than 5% for commercial product and nano-formulation. Similar results were obtained for volatilization tests from soils (30% lost from soils treated with pure dicamba to approximately 5% lost from soils treated with the commercial dicamba-based product and the nano-formulation). Transport tests were performed injecting in sand-packed columns the herbicidal formulations diluted both in DIW and tap water. Pure dicamba and the commercial herbicide showed no retention within the columns, reaching 100% recover at the outflow of 15 cm-long columns, both in saturated and unsaturated conditions. For the nano-formulation, the maximum recovery was 30% in unsaturated conditions, and 60% in saturated columns, with minimal recovery in most tests for both conditions. The column tests results were modeled using colloid transport software (namely MNMs and Hydrus) and used for the development of a preliminary field-scale simulation of herbicide application and dispersion in the subsoil. The work was developed in the framework of the project Nanograss, co-funded by Compagnia di San Paolo Foundation.

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A Numerical Study on Multiphysics Fluid Flow in a Shale Gas Reservoir with Non-Uniform Fractures

Authors: Abhishek Kumar[1]; Suresh Kumar Govindarajan[2]

[1] *Research Scholar, Reservoir Simulation Laboratory, Petroleum Engineering Program, Department of Ocean Engineering, Indian Institute of Technology, Madras, Chennai 600036, India.*

[2] *Professor, Reservoir Simulation Laboratory, Petroleum Engineering Program, Department of Ocean Engineering, Indian Institute of Technology, Madras, Chennai 600036, India.*

Corresponding Authors: gskumar@iitm.ac.in, abhikumar2106@gmail.com

The last decade has shown an increasing trend for the exploitation of oil and gas from unconventional reservoirs resulting because of the depletion in conventional oil and gas resources. The advent of hydraulic fracturing and horizontal drilling has led to the development of shale gas reservoirs which constitutes a major portion of such reservoirs. Shale reservoirs have very low permeability with ultra-small pores with low connectivity. The gas is stored as free gas inside the shale matrix pores as well as in the fractures and as adsorbed gas on the surface of the organic matter in the shale matrix. Fractures aid in the migration of gas from these reservoirs. The depletion in shale gas reservoirs leads to a decrease in reservoir pressure and adsorbed gas gets desorbed from the organic matter. This depletion also leads to a change in porosity and permeability within the reservoir. Desorption of adsorbed shale gas from the solid grain surfaces within the low permeable shale matrix is defined using Langmuir isotherm. Following the desorption of shale gas into the pores, the fluid migration within the low permeable shale matrix is described by unconventional diffusive methods such as Knudsen diffusion and Surface diffusion based on the pore sizes of the low-permeable shale-matrix. The shale gas then gets transported to the relatively high permeable fractures from the low

permeable shale matrix. The mobility of shale gas is generally modeled using a simplified uniform fracture with a constant fracture aperture thickness. However, in reality, these fracture apertures will not be uniform along the fracture length and eventually makes the resultant fluid flow to be non-uniform. Thus, the present work focuses on numerical simulation of multi-physics fluid flow in a stress-sensitive shale gas reservoir consisting of non-uniform fractures. The non-Darcy flow within the high permeable fractures is taken into account by using an apparent permeability concept. The stress-sensitivity of porosity and permeability in the shale matrix as well as the fracture is also taken into account considering the role of coupled fluid flow and geo-mechanics. A dual-porosity model has been applied in order to simulate the coupled fracture-matrix fluid mass fluxes. In addition, we have investigated the effect of stress-sensitivity on pressure, porosity, and permeability. The present model aims to study the stress-sensitive nature of a shale gas reservoir with non-uniform fracture apertures and its impact on the resultant recovery of shale gas. Finally, the study of the present numerical model results with respect to the dimensional properties has been investigated.

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The hydraulic conductivity of shaped fractures with permeable walls

Authors: Daihui Lu[1]; Federico Municchi[2]; Ivan Christov[1]

[1] *Purdue University*

[2] *University of Nottingham*

Corresponding Authors: federico.municchi@gmail.com, christov@purdue.edu, lu565@purdue.edu

Whether natural or induced, underground fractures have non-uniform shapes 1. Their cross-sectional area generally decreases slowly in the direction of the flow through the fracture [2,3]. The walls of the fracture are the surrounding geological porous rock formations [4]. Thus, fluid can leak from the fracture into the surrounding rock matrix. This leakage has significant implications for oil and gas recovery, as well as for evaluating the safety of groundwater reserves residing near fractures. What has not been appreciated in previous studies of flow in fractures is just how the fluid flow into the permeable walls is determined by the rocks' properties, the varying fracture geometry, and the pressure forces driving the flow.

In this study, we investigate the flow-wise variation of the hydraulic conductivity inside a non-uniformly shaped fracture within a porous medium. Using lubrication theory for viscous flows, in conjunction with the Beavers–Joseph–Saffman boundary condition [5,6] at the permeable walls, we obtain an analytical expression for the conductivity. This prediction highlights the effects of geometric variation (through the local slope of the aperture's flow-wise variation), the permeability of the walls (through a dimensionless slip coefficient), and the effect of flow inertia (through a Reynolds number). The theoretical results are validated against an OpenFOAM solver for the Navier–Stokes equations (based on the SIMPLE algorithm) subject to the tensorial Beavers–Joseph–Saffman boundary condition, showing good agreement.

This study contributes and validates a mathematical expression for the resistance to flow in a single fracture, elucidating analytically the coupled roles of shape variation and permeation into the walls. Having such a precise prediction in hand can improve systems-level modeling of complex transport phenomena through (hydraulically) fractured rock, which guides the evaluation of the lifespan of an oil or gas reservoir and the efficacy of underground carbon dioxide sequestration, amongst other applications. For example, in system-level (and multiscale) modeling, the Darcy conductivity of each non-uniform passage must be accurately accounted for throughout a fractured porous rock.

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1308

A novel molecular communication paradigm for porous media applications

Authors: Matteo Icardi[1]; John Couch[1]

[1] *University of Nottingham*

Corresponding Author: matteo.icardi@nottingham.ac.uk

Molecular communication (MC) is a relatively new type of communication which makes use of particles to transmit information. The idea of moving towards particle transfer over classical waveform transfer is appealing as it broadens the range of what we are able to communicate through (more) efficiently, such as porous mediums. MC systems also have a wide range of applications, such as medical treatments using smart drugs, its potential of active sensing in nanotechnology, and also in improving industrial problems such as how to obtain reliable data from chemical reactions. In this paper, we combine fluid mechanics and communication theory with the aim to understand MC in a mathematical framework. This approach is still in its infancy, and so we aim to progress this viewpoint by providing a solid mathematical basis which can be used for future research in this field, or fields alike. To begin with this aim, we start from the fluid mechanical perspective by studying simple one-dimensional transport models, and use ideas from communication theory such as transmission, modulation, reception, and demodulation, to find an optimal way of sending information across a porous medium. To achieve this, we use the transfer function (arrival time distribution) obtained from the transport operator and develop signal carrier/modulating functions, as set of orthogonal/bi-orthogonal functions, found via Singular Value Decomposition (SVD) of the discretised operator. These are proven to be the optimal way for sending information but require the definition of negative signal, that can be achieved by the transport of multiple species. Once a communication scheme is developed, the channel capacity can be numerically evaluated using Shannon's mutual information concepts.
This novel framework may lead to promising results in nanosensing applications as well as optimal injection strategies for forward and inverse uncertainty quantification, when applied to an uncertain or stochastic media. This idea is tested in three-dimensional random media where the response function is estimated by solving the transport problems in the frequency domain.

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Multiple Retention Mechanisms during Transport in Porous Media: Numerical modelling and empirical parameters evaluation

Authors: Jocenrique Carlo de Oliveira Rios[1]; Adriano dos Santos[1]; Sidarta Araújo de Lima[1]

[1] *Universidade Federal do Rio Grande do Norte*

Corresponding Authors: adriano_stos@yahoo.com.br, sidarta@lncc.br, jocenrique@ufrn.edu.br

Understanding transport and retention in porous media is essential in environmental and industrial processes like aquifer contamination, water and polymer flooding in petroleum reservoirs, etc. In this work, population balance equations for transport and retention are discussed based on Master Equation 1. The obtained system of equations consists of one retention and one population equation for each class of particles. Averaging the aforementioned equations results in a system consisting of an advection-dispersion-reaction equation and the retention kinetics. In addition, accounting for the permeability reduction due to retention mechanisms, the modified Darcy's law 2 is coupled to the aforementioned system. The result is a closed system of equations for modeling both retention and formation damage during flow and transport in porous media. In addition, an accurate and robust numerical solution based on KT (Kurganov-Tadmor) finite volume method 3 is proposed and validated by comparing it with analytic solutions [4, 5]. Transport and retention parameters are optimized by fitting experimental data available in the literature. Good agreement between proposed model and experimental data was observed, and allowed concluding that an accurate set of parameters is obtained if pressure drops, and suspended and retained concentrations are simultaneously fitted. Finally, it was shown that transport and retention coefficients (including dispersion coefficient) can be simultaneously obtained by numerically solving the inverse problem for any effluent concentration data, suggesting that the traditional tracer injection [6, 7] is not necessary in order to determine the hydrodynamic dispersion coefficient.

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1310

The first nanoremediation pilot-test in Brazil: site selection criteria and nZVI mobility studies

Authors: Daphne Silva Pino[1]; Reginaldo Bertolo[1]; Petr Kvapil[2]; Carlo Bianco[3]; John Etim[4]; Tannaz Pak[4]

[1] *University of Sao Paulo, Brazil*

[2] *Photon Water, Tchec Republic*

[3] *University of Turin, Italy*

[4] *Teesside University, United Kingdom*

Corresponding Authors: t.pak@tees.ac.uk, petr.kvapil@photonwater.com, daphne.pino@usp.br, carlo.bianco@polito.it, bertolo@usp.br, w9025087@tees.ac.uk

More than two billion people rely on groundwater as their primary water source. Groundwater contamination is a major global problem which can cause significant health issues for communities relying on it. We present the results of the first phase of a collaborative multi-disciplinary and multi-country research project, that aims to perform the first pilot-scale nano-based groundwater remediation (nanoremediation) project in Brazil. Our work is focused on the state of Sao Paulo which has significant groundwater problems due to industrial activities and population growth1. Since 2002, the state environmental agency publishes a registry of contaminated areas, annually, to inform the public of the actions carried in those areas2. The registry provides a summary of the data from consulting companies reports acquired during site management phases, portraying the site conditions updated at the end of each year for thousands of contaminated areas.

The target of this work is to prepare for and carry out subsurface injections of nanoscale zero valent iron particles (nZVI) within a selected aquifer known to be contaminated with chlorinated solvents, which are among the most persistence groundwater contaminants3. To achieve this, we studied 10 major contaminated sites in the State of Sao Paulo. We have used the databases published by the environmental agency to select these areas to consider for this pilot study. A set of criteria was developed based on previous successful pilot/field applications of nZVI remediation to assist with the selection of the site most suitable for using nanoremediation technology, through performing a mapping exercise.

The key criteria considered were: (i) quality of the existing site description, as more robust conceptual site models will result in design of more effective nanoremediation processes; (ii) availability of previous tracer tests to aid defining the hydraulic connections between the injection and the monitoring wells; (iii) type of contamination and concentration levels; (iv) total volume of the contamination; and (v) water salinity, as nanoremediation can be applied where water salinity is in the order of ppm (or mg/L), however, if it reaches thousands of ppm (or g/L), the technology becomes limited as both the life span of the nanoparticles and the particle mobility will be reduced.

The two selected sites are different considering: (i) the amount, type, and distribution of contamination currently present at each site, and (ii) the available data and equipment, given previous remediation activities/studies carried out at each site. The following step was investigating the mobility of nZVI in each site using the MNMs software[4]. Based on site-specific hydrogeological information, the nZVI injection through a screened well (radial geometry) is simulated in each site to estimate the expected radius of influence and final particle distribution within the aquifer. A sensitivity analysis is then performed to determine the best set of operating parameters (e.g. injection flowrate, well size and screened length, particle concentration) to be applied for an effective iron delivery. The comparison of the results in terms of expected particle mobility will allow to finally choose the optimal site for this pilot-scale nanoremediation application.

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Pore scale observations of wetting alteration during low salinity water flooding

Author: Edward Andrews[1]

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

[1] *Imperial College London*

Corresponding Authors: a.muggeridge@imperial.ac.uk, epa114@ic.ac.uk, s.krevor@imperial.ac.uk

Low salinity water flooding has been shown to increase oil recovery both on the core and field scale in many but not all sandstones. Both macro scale and sub pore scale observations suggest that lowering the salinity of injected water can alter the wetting state of the rock, usually making it more water-wet. However, there remains a poor understanding of how wettability alteration at the microscopic scale leads to oil redistribution and recovery at core and field scales.
In this work, X-ray micro-CT scanning is used to image unsteady state experiments of tertiary low salinity water flooding in two Berea sandstone cores. The wetting state of one of the cores was altered with exposure to crude oil. In the unaltered rock, oil was trapped at a saturation of 0.74 after high salinity water flooding. This did not change significantly after subsequent flooding with low salinity brine. In contrast, in the altered sample, oil was trapped more heterogeneously and at relatively low oil saturation of 0.62 after high salinity flooding. Subsequent flooding with low salinity brine resulted in a three percentage point oil production. In the altered sample, we observe a shift in the solid surface area covered by the oil phase after low salinity water flooding consistent with a change from an oil-wetting to a less oil-wetting state. This change is also reflected in the observed variation in fluid pore occupancy. As a result of the shift in wetting state, 22% of oil originally in place was mobilised during low salinity flooding. However, only a fifth of this mobilised oil was produced - the rest was re-trapped. We find that the success of low salinity water flooding depends on both the ability of low salinity brine to alter the wetting state to more water-wetting and the pore structure to facilitate the production of mobilised oil.

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A new generation of lattice Boltzmann code for pore-scale simulation of scCO2-brine displacement in complex geometries

Authors: Yu Chen[1]; Qinjun Kang[2]; Albert Valocchi[3]; Hari Viswanathan[2]

[1] *Los Alamos National Lab*

[2] *Los Alamos National Laboratory*

[3] *Univ Illinois*

Corresponding Authors: viswana@lanl.gov, qkang@lanl.gov, yu_chen@lanl.gov, valocchi@illinois.edu

Direct numerical simulation (DNS) of flow in porous media plays an increasingly important role in understanding pore-scale flow physics and obtaining constitutive parameters for upscaling, owing to the rapid development of X-ray tomographic imaging techniques and modern high-performance computing. Our recent study(Chen et al., 2019) shows that inertial effects, which can be represented by Ohnesorge number (Oh), must take into consideration during the scCO2-brine displacing process in real rock geometry. However, matching the Oh of a physical scCO2-brine flow system imposes a requirement on the ratio of viscosity over surface tension, where many traditional models either cannot fulfill this requirement or cannot perform practical 3D simulations on real rock samples due to the computational cost from using complex algorithms.

In this work, we introduce our in-house developed "MF-LBM-v2"code, which employs the continuum-surface-force (CSF) based color-gradient lattice Boltzmann (LB) multiphase model and geometrical wetting model to reduce spurious currents and eliminate artificial films, thus enables us to match the inertial effects of the physical scCO2-brine system. The code is validated against simple benchmarks as well as the experimental data of liquid CO2 displacing water in a heterogeneous micromodel under reservoir pressure conditions. The code is highly optimized for manycore processors/co-processors, and achieves significant speedup compared to traditional CPU, which enables us to perform pore-scale simulations on real rock samples under realistic conditions. We will present the performance data of the code on different computing platforms. Despite that the advanced models increase the computation cost of each iteration, our present code is up to three times faster than the code based on a traditional LB model in actual computing time, thanks to the increased numerical stability so that larger physical time step can be used.

Finally, we employed the code to perform high-fidelity DNS on a Bentheimer sandstone sample to show the inertial effects under different wetting conditions. In addition, we performed a core-scale drainage DNS (video of the core-scale DNS) at Ca=2×10^(-6) , using 2.6 billion grid points to demonstrate the capability of the code and also to evaluate the consistency between the entire core simulation and simulations with smaller domain.

Chen, Y. et al. (2019), Water Resources Research, 55(12), pp. 11144–11165. doi: 10.1029/2019WR025746.

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: Numerical predictive modelling for groundwater remediation using nanotechnology.

Authors: Daphne Silva Pino[1]; Tannaz Pak[2]; Alexander Wood[2]; Masoud Babaei[3]; Reginaldo Bertolo[4]

[1] *Groundwater Research Centre (CEPAS-USP)*

[2] *Teesside University*

[3] *Manchester univeristy*

[4] *University of Sao Paulo, Brazil*

Corresponding Authors: t.pak@tees.ac.uk, alexander.wood@tees.ac.uk, daphne.pino@usp.br, bertolo@usp.br

Successful remediation of contaminated groundwater resources is known to have many barriers1. These limitations are more significant for ex-situ techniques compared to in-situ ones. An ex-situ technique such as excavation of contaminated soil for landfill or incineration, although a move toward total contaminant removal, poses a risk to business disruption. For the two candidate contaminated sites we are studying the source and plume locations are situated within operating facilities of active businesses. A halt in production (needed for a safe soil excavation and removal) presents a scenario with concerning socio-economic impacts to local business. In-situ remediation techniques address spatial disadvantages as they do not require removal of contaminated soil for remediation. Instead, injection of reactive material (chemicals or particles) offer a remediating solution addressing the contaminated area in-situ. In-situ remediation can be achieved through chemical degradation. However, in-situ chemical oxidation of chlorinated solvents using potassium permanganate can cause formation of a precipitate resulting in reduction in fluid mobility within the pore structure.

Nanoscale zero valent iron (nZVI) is an emerging technique within in-situ remediation. Nanoremediation is an attractive proposition as it has been shown to improve reaction time due to a large surface area when compared to microscale zero valent iron. This reaction rate is especially an advantage when compared to bioremediation. Remediation by nZVI is effective for a range of contaminants, including chlorinated solvents. The goal of this study is to study the application of nanoremediation technology for in-situ degradation of chlorinated solvents in two contaminated sites in Brazil. This technology is chosen based on the small footprint for nZVI injection, reducing the invasiveness of this technique.

The two contaminated sites we study are located in the outskirts of the city of Sao Paulo. A pore-scale study has recently shown that nanoremediation can cause remobilisation of previously trapped droplets of chlorinated solvents2. Building on this study we are using field-scale 3D aquifer models (constructed in PetraSim software) to solve multiphase flow in porous media to focus on contamination transport in these two groundwater systems. 3D models were built based on cross sectional maps and data (e.g. hydraulic conductivity and porosity) extracted from publicly available environmental reports. These models are used to study the (i) preferential flow pathways through the contamination source and plume for each site induced and exacerbated by heterogeneity of the aquifer system, and (ii) the viscous displacement of the trapped contaminant as a function of nZVI concentration that leads to varying degree of piston-like displacement.

This study offers the opportunity to model and explore the difference in tropical soil and high levels of rainfall have on groundwater contamination and how remediation may need to be adjusted to account for this.

The outcomes of this work inform a pilot-scale nanoremediation project, currently at the design stage, as part of the GRUN project (UK-Brazil collaborative research). Performing these sensitivity analysis on the key parameters contributing to a successful process at the field scale. This will enable us to identify the most suitable site(s) for effective application of nanoremediation.

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Estimating Oil Recovery Factor from Reservoir Characteristics using the XGBoost Algorithm

Author: Alireza Roustazadeh[1]

Co-authors: Behzad Ghanbarian [1]; Mohammad Shadmand [2]; Vahid Taslimitehrani [3]; Larry Lake [4]

[1] *Porous Media Research Lab, Department of Geology, Kansas State University, Manhattan, 66506, KS, USA*

[2] *Department of Electrical & Computer Engineering, Kansas State University, Manhattan, KS*

[3] *Vahid Taslimitehrani, PhD Senior Machine Learning Scientist, realtor.com Santa Clara, CA*

[4] *Department of Petroleum and Geosystems Engineering, University of Texas at Austin, Austin, 78712, TX, USA*

Corresponding Authors: aroustazadeh@ksu.edu, mshadmand@ksu.edu, ghanbarian@ksu.edu, larry_lake@mail.utexas.edu, taslimi.vahid@gmail.com

Abstract

Accurately estimating oil recovery factor can save the exploration industry millions of dollars. Although oil recovery factor can be determined with relatively good accuracy at small core scales, its estimation at the reservoir scale is still a major challenge for oil and gas companies because of large-scale heterogeneities and complexities.

With recent advances in machine learning algorithms, it is possible to analyze large databases even with missing data. If imputation and training algorithms are optimized, results can greatly improve the quality and accuracy of recovery factor estimation. The main objective of this study was to estimate the oil recovery factor from reservoir characteristics, such as porosity, permeability and lithological properties using a large commercial database including nearly 1,200 reservoirs from all around the world. First, we cleaned up the database by removing samples whose oil recovery factors were missing. This decreased the number of samples to almost half. Then, we imputed the missing data using a new algorithm. For this purpose, the remaining oil recovery factor data were sorted from the smallest to the largest. After that, subclasses of data including at least 10 samples with less than 10% of missing data were used to find the mode from the histogram of each input parameter. The missing data were then replaced with the modes in the corresponding oil recovery factor subclass. After the imputation, we applied the Tree Based Gradient Boost model (XGBoost) to train and test the model. For the training and test samples, after 1000 iterations, we found the average RMSLE = 0.067 and 0.086 and R2 = 0.78 and 0.64, respectively. Comparing the determined R2 values with those reported for some existing models developed for databases with similar diversity showed a significant improvement in the estimation of oil recovery factor at the reservoir scale.

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A multi-step Dirichlet-Neumann domain decomposition method applied to the polymer injection in porous media

Authors: Renatha Batista dos Santos[1]; Rodrigo Silva Tavares[1]; Sidarta Araújo Lima[1]; Adriano Santos[1]

[1] *Universidade Federal do Rio Grande do Norte*

Corresponding Authors: adriano@eq.ufrn.br, rodstavares1@gmail.com, renathabat@gmail.com, sidarta@ccet.ufrn

The flow and particle transport in porous media have been extensively studied due to its industrial and scientific applications. Various mechanisms, such as diffusion, sedimentation, interception, straining, adsorption, and swelling are responsible for the pore blocking and formation damage in porous media 1. In particular, during polymeric solutions flow (non-Newtonian fluid) in porous media, mechanical retention and adsorption phenomena can occur giving rise to formation damage and injectivity loss.

In this work, we propose new computational modeling based on multiple time steps domain decomposition technique together with the Dirichlet-Neumann method applied to the numerical simulation of non-Newtonian fluids hydrodynamic and polymer transport on porous media. We consider that the flow of a pseudo-plastic polymeric solution is quantified by a non-linear Darcy's law, at which the injected fluid viscosity depends on the polymer concentration and shear rate based on Carreau's Law 2. Furthermore, the polymer movement is quantified making use of a convection-diffusion-reaction transport equation where a reactive term arises due to mechanical retention and adsorption 3. The proposed model also takes into account the formation damage by postulating the porosity and permeability as a function of the polymer concentrations retained and adsorbed.

From the computational point of view to coupling the near well phenomena with the porous media, we apply the Multi-timestep Dirichlet-Neumann domain decomposition method [4]. Such a scheme employs different temporal steps in the time decomposition together with the classical spatial decomposition based on the Dirichlet-Neumann method. The main feature of the method is the coupling of the time decomposition based on a Predictor-Corrector strategy. Then, the non-linear mathematical model is discretized in each subdomain making use of the finite element method together with the Newton-Raphson method 5. The kinetic law for mechanical retention is post-processed by the Runge-Kutta method.

Finally, we propose some numerical simulations comparing the discrete solutions with analytical and high fidelity solutions to analyze the efficiency and low computational cost of the domain decomposition method in capture the near well/porous media phenomena with accuracy. The main goal of this work is to simulate numerically the coupling between formation damage, non-Newtonian flow, and loss of injectivity during polymer injection in porous media considering perforated wells.

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Effect of grain-size distribution on the temporal evolution of interfacial area during multi-phase flow through porous media

Author: Fizza Zahid[1]

Co-authors: Jeffrey A. Cunningham [1]; Amy Stuart [1]

[1] *University of South Florida*

Corresponding Authors: cunning@usf.edu, als@usf.edu, fizzazahid@usf.edu

During multi-phase flow in porous media, mass transfer mechanisms take place at the interface of the two fluids. Therefore, interfacial area is an important factor in the fate and transport of the fluids. The development of interfacial area over time may depend on the porous medium's properties such as grain morphology, pore connectivity, and/or grain-size distribution. The objective of this work is to quantify how grain-size distribution affects the temporal development of interfacial area during multi-phase flow through porous media. A multiphase lattice Boltzmann model (LBM), using the color gradient method (Guntensen et al., 1991; Reis and Phillips, 2007), is used to simulate oil and water drainage and imbibition in an ensemble of two-dimensional porous media samples (Mollon and Zhao, 2012). We conducted simulations on 3 groups of porous media: a group of 20 well sorted realizations (coefficient of uniformity = 1.2), a group of 20 intermediate realizations (coefficient of uniformity = 1.5), and a group of 20 poorly sorted realizations (coefficient of uniformity = 1.8). Each of the 60 realizations were conducted for 1×10^6 LBM time steps, and the interfacial area was monitored after every 500 time steps. We observe that the peak interfacial area occurs when the defending fluid is at 0.20-0.30 for drainage and imbibition, regardless of grain-size distribution. During drainage, the overall trend for all three groups is that the interfacial area increases until a peak is reached, starts decreasing and then acquires a plateau status. On average, the poorly sorted realizations reach the peak interfacial area earlier than the intermediate or well sorted realizations during drainage. During imbibition, the peak interfacial areas are higher than seen in drainage for all three groups. The results indicate that grain size distribution affects the interfacial area development, particularly in terms of the time at which the peak interfacial area is reached. Based on the rapid development of interfacial area in the poorly sorted media, it is reasonable to estimate that inter-phase mass transfer would occur more rapidly in these soils. This implies, for instance, that remediation of oil spills via technologies that depend on inter-phase mass transfer might act more rapidly in poorly sorted soils than in well sorted soils. Hence, the results of this work can help understand and improve groundwater and soil remediation efforts, e.g., by helping to select remediation strategies that are best suited for the soil under consideration.

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1319

Nonlocal nonlinear upscaling for problems in heterogeneous and fracture media using machine learning technique

Author: Maria Vasilyeva[None]

Co-authors: Eric Chung [1]; Yalchin Efendiev [2]; Tat Leung Wing [3]

[1] *The Chinese University of Hong Kong*

[2] *Texas A&M, USA*

[3] *Department of Mathematics, University of California, Irvine*

Corresponding Authors: wtleung@uci.edu, efendiev@math.tamu.edu, tschung@math.cuhk.edu.hk, vasilyevadotmdotv@gmail.com

In this work, we present the nonlocal nonlinear upscaling method for problems in heterogeneous and fracture media. We construct an upscaled coarse grid model using a machine learning technique. The

proposed upscaled model is based on the solution of the local problem in the oversampled domain up to fine grid resolution that used to create an accurate dataset for the training of the neural networks. We present numerical results for several applications in heterogeneous and fractured media: (1) unsaturated flow, (2) two-phase flow, and (3) poroelasticity problem. Our numerical results show that the proposed approach can provide very good accuracy with fast calculations.

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Modeling and design optimization for pleated membrane filter

Authors: Yixuan Sun[1]; Pejman Sanaei[2]; Lou Kondic[1]; Linda Cummings[1]

[1] *NJIT*

[2] *NYIT*

Corresponding Author: ys379@njit.edu

Pleated membrane filters, which offer larger surface area to volume ratios than unpleated membrane filters, are used in a wide variety of applications. However, the performance of the pleated filter, as characterized by a flux-throughput plot, indicates that the equivalent unpleated filter provides better performance under the same pressure drop. Earlier work (Sanaei & Cummings 2016) used a highly-simplified membrane model to investigate how the pleating effect and membrane geometry affect this performance differential. In this work, we extend this line of investigation and use asymptotic methods to couple an outer problem for the flow within the pleated structure to an inner problem that accounts for the pore structure within the membrane. We use our new model to formulate and address questions of optimal membrane design for a given filtration application.

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1321

Experimental Investigations of Oil Transport in 2D Porous Media

Authors: Jiwei Wu[None]; Thomas Cochard[1]; Lizhi Xiao [2]; David A. Weitz[3]

[1] *Harvard University*

[2] *China University of Petroleum Beijing (CUPB)*

[3] *Harvard University, USA*

Corresponding Authors: th.cochard@gmail.com, weitz@seas.harvard.edu, xiaolizhi@cup.edu.cn, jiweiwu@g.harvard.edu

The understanding of immiscible flow in porous media is a major interest for oil and gas recovery in conventional reservoir. Many people try to compare different rocks, fluids and surfactants, but that' s hard to establish a deep understanding. In order to understand how the oil is being transported in such condition, we generate an artificial 2D porous media. Those artificial porous materials are then transferred into a PDMS chip. With visualization, we might be able to figure out the structural features that dictate different pinch-off mechanisms. Coupled with high speed imaging we can track the initial oil ganglia, look at its transport which can be achieved in several ways: continuous transport, break up into smaller ganglia but also study the coalescence of oil ganglia under certain conditions. New way of modelling the transport behavior are proposed and a framework of modelling the tertiary oil and gas recovery is suggested.

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Multiscale model reduction of unsaturated flow problem

Author: Denis Spiridonov[1]

Co-authors: Maria Vasilyeva [2]; Eric T. Chung [3]; Yalchin Efendiev [4]

[1] *Multiscale model reduction laboratory, North-Eastern Federal University, Yakutsk, Republic of Sakha (Yakutia), Russia, 677980*

[2] *Institute for Scientific Computation, Texas A&M University, College Station, TX 77843-3368 \& Department of Computational Technologies, North-Eastern Federal University, Yakutsk, Republic of Sakha (Yakutia), Russia, 677980*

[3] *Department of Mathematics, The Chinese University of Hong Kong (CUHK), Hong Kong SAR*

[4] *Department of Mathematics \& Institute for Scientific Computation (ISC), Texas A&M University, College Station, Texas, USA*

Corresponding Authors: efendiev@math.tamu.edu, eric.t.chung@gmail.com, d.stalnov@mail.ru, vasilyevadotmdotv@gmail.com

In this work, we consider a multiscale method for simulations of the multicontinua unsaturated flow problems in heterogeneous fractured porous media. We present fine grid approximation based on the finite element method and Discrete Fracture Model (DFM) approach. In this model, we construct an unstructured fine grid that takes into account complex fracture geometries for two and three dimensional formulations. Due to construction of the unstructured grid, the fine grid approximation leads to the very large system of equations. For reduction of the discrete system size, we develop a multiscale method for coarse grid approximation of the coupled problem using Generalized Multiscale Finite Element Method (GMsFEM).

In GMsFEM, we construct coupled multiscale basis functions that are used to construct highly accurate coarse grid approximation.
We also consider case with rough surface topography. To treat rough boundaries, we construct additional basis functions to take into account the influence of boundary conditions on rough surface. We investigate accuracy of the proposed method for the several test problems in two and three dimensional formulations. Numerical results illustrate that the presented method provides accurate solution of the unsaturated filtration problems on the coarse grid with huge reduction of the discrete system size.

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Stochastic Modelling of Adsorption and Sieving in a Pore Network

Authors: Binan Gu[1]; Pejman Sanaei[2]; Linda Cummings[3]; Lou Kondic[3]

[1] *New Jersey Institute of Technology*

[2] *NYIT*

[3] *NJIT*

Corresponding Author: bg263@njit.edu

We formulate the membrane filtration process in a random network where vertices and edges of the underlying graph represent pore junctions and throats. We study the adsorptive and sieving fouling mechanisms simultaneously and define each mode rigorously. The main goal is to relate membrane filter material and physical properties to the performance of the filter, using tools from spectral graph theory. We also provide a formula for network tortuosity in terms of the adjacency matrix of the representative graph and the transition matrix of a sieving particle which we assume to perform a weighted random walk on the network.

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The effects of oxidation on the capacity of shale gas desorption and diffusion in nanoscale pores

Authors: Yang Zhou[1]; Lijun You[1]; Yili Kang[1]; Qiuyang Cheng[1]; Yang Chen[1]

[1] *Southwest Petroleum University*

Corresponding Author: zhouy2020@126.com

The multi-scale fractures formed by hydraulic fracturing provide transport channels for shale gas production. However, the gas in shale nanopores is mainly produced by diffusion, and the gas supply capacity is far lower than the gas flow capacity in fractures, resulting in a rapid production decline. During the development of shale gas reservoirs, the fluids used for fracturing is exposed to air for a long time, which usually contained a large amount of dissolved oxygen(8.0~9.0 mg/L). As a result, a large amount of oxygen enters the shale reservoir with the fracturing fluids. As organic-rich shale is usually formed in anoxic sedimentary environment, it is rich in organic matter and reductive minerals (such as pyrite chlorite). The reductive minerals are easy to react with dissolved oxygen by oxidation, releasing a large number of SO42- and Fe3+, which is easy to produce iron-bearing precipitation and insoluble sulfate precipitation, thus inducing the blocking of shale nanopores and damaging the diffusion capacity of shale gas. By observing the field emission scanning electron microscope (FESEM) images of shale after contact with dissolved oxygen, the damage capacity of oxidation to nanopore was confirmed, and the damage degree of oxidation to shale gas diffusion capacity was 54.5% through the test of gas diffusion coefficient.
This article explored the new method of oxidative fracturing to solve the damage of dissolved oxygen. By adding oxidizing fluid to the hydraulic fracturing fluids, the method can not only break shale with the hydraulic fracturing technology, but also break shale with the oxidation reaction. A large number of fracturing fluids are retained to allow sufficient reaction time and space for oxidizing fluids, which is the engineering basis for the implementation of oxidative fracturing.
The proportion of adsorbed gas in shale is 20%~85%. The adsorbed gas mainly occurs in the organic nanopores. The transport mechanism of the adsorbed gas is mainly desorption-diffusion and slippage flow. Compared with the free methane in larger scale space, the adsorption gas has lower production rate and production degree.
During oxidative fracturing, the organic matter is consumed in large quantities, which can greatly reduce the ability of shale gas adsorption. Meanwhile, oxidation reaction can also generate lots of heat. Under the influence of these two effects, the desorption capacity of adsorption gas in shale nanopores is improved. Large amounts of organic matter and pyrite are dissolved by oxidation reaction, which will produce large number of dissolved pores and fractures, improve the gas supply capacity of the pore throat of the shale block to the fracture system, induce the expansion and extension of shale micro-fractures, shorten the gas transport path in the shale block, so as to relieve the damage of dissolved oxygen and improve the recovery rate of shale gas reservoirs.

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1326

Pore network modeling of fuel cell catalyst layer performance

Author: Amin Sadeghi[None]

Co-authors: Shawn Litster [1]; Jeff Gostick [2]

[1] *Carnegie Mellon University*

[2] *University of Waterloo*

Corresponding Authors: amin.sadeghi@uwaterloo.ca, jgostick@uwaterloo.ca

A deeper understanding of pore-scale processes in fuel cell catalyst layer is key to optimizing its performance, reducing its cost, and ultimately making the fuel cell technology more affordable. A major challenge in doing so is the multiscale nature of the catalyst layer which ranges from only a few nanometers in ionomer films up to a few hundred nanometers in intra-agglomerate pores. This huge difference in length scales leads to significant computational costs if conventional pore-scale modeling approaches such as direct numerical simulation were to be employed. Following our previous works [1-2], here we present a multiphysics pore network model that accounts for the different physics and length scales present in the catalyst layer while being able to capture the pore-scale phenomena reasonably accurately. The pore network model was extracted from real tomography data using the SNOW algorithm 3. The use of the network modeling approach enabled us to perform the simulation on a relatively large domain of the catalyst layer that is otherwise inaccessible to probe using conventional pore-scale modeling approaches.

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1327

Role of Temperature on Threshold Gradient and Permeability of non-Darcian Flow in Sand and Clay Mixtures

Authors: Yuntian Teng[1]; Zihao Li[1]; Weiyu Zheng[1]; Yifeng Wang[2]; Rui Qiao[1]; Cheng Chen[1]

[1] *Virginia Polytechnic Institute and State University, Blacksburg, VA, United States*

[2] *Sandia National Lab, Albuquerque, NM, United States*

Corresponding Authors: ruiqiao@vt.edu, weiyu@vt.edu, chen08@vt.edu, zihao91@vt.edu, yteng@vt.edu

The swelling of clay results in the non-linearity at the lower pressure range of the relationship between water flow velocity and the pressure gradient. A threshold gradient exists for triggering the flow in the low-permeability porous media which is of vital importance in unconventional hydrocarbon recovery and radioactive waste disposal. In this study, experiments of 0.1M ionic strength NaCl solution flowing through mixtures of 10% clay and 90% sand columns are performed to measure the

permeability and threshold gradients at temperatures ranging from 20℃ to 90℃. The non-linear parts of the flow velocity and hydraulic gradient curves are also measured and plotted to exhibit the process. The experiments are based on a customized core flooding system designed for high-precision measurement of hydraulic gradient and permeability of swelling bentonite. The liquid permeability and the threshold gradient are measured in a steady-state flowing condition by a high-precision differential pressure transducer connected to the ends of the column, as well as a high-precision flow meter. Experimental results show that the relationship between permeability and threshold gradient is a power-law correlation, as proposed by Birkholzer and Liu 1. The results also indicate that higher temperatures lead to lower threshold gradients, as predicted by the continuum-scale two-parameter model for non-Darcian flow in low permeability porous media proposed by Chen 2. The power-law relationship of permeability and threshold gradient at higher temperatures have smaller constants which reveal a left lower movement of the curves with higher temperatures, as indicated by the Chen model. This study takes advantage of a customized core flooding experimental system to investigate the role of temperature on the threshold gradient of non-Darcian flow in low permeability porous media.

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1328

Integration of Pulse Decay Experimental Data into a Novel Continuum-Scale Multi-Physics Model to Study Gas Transport in Shale Formations

Author: Zihao Li[1]

Co-authors: YUNTIAN TENG ; Ming Fan [1]; Cheng Chen [2]

[1] *Virginia Tech*

[2] *Department of Mining and Minerals Engineering, Virginia Tech, Blacksburg, Virginia, USA.*

Corresponding Authors: mingfan@vt.edu, yteng@vt.edu, zihao91@vt.edu

Investigation about gas transport in the shale reservoirs is challenging since the transportation process is dominated by multi-physics mechanisms. The apparent permeability and absolute permeability of the shale reservoir have a significantly different because of the Klinkenberg effect in the shale nanopores. The effective stress on the shale also has a great impact on the apparent permeability of the shale formation. In this study, a modified dual-porosity-permeability model was introduced to investigate shale gas transport. The model includes two domains, an organic matter (kerogen) domain, and an inorganic matrix. Each domain has its own permeability, porosity, compressibility, etc. Under a pressure gradient, the viscous flow governs gas transport in the domains. The mass exchange between two domains is described by a coefficient called the mass-exchange-rate coefficient. These two domains are imposed on external confining pressure simultaneously. The actual effective stress on the model is obtained by the external confining pressure and internal pore pressure by considering Biot's coefficients. The relationship between apparent permeability and effective stress is developed through this model. To validate this novel model, the permeability of shale samples from two U.S. shale reservoirs were measured by a pulse decay permeameter (PDP) with multiple groups of pore pressure and confining pressure. The values of the Biot's coefficient were calculated

by the experimental data. Sensitivity analysis was also conducted to illustrate the weight of each input variable on the final output variable. The results show the modified dual-porosity-permeability model can fit the curves from experimental external-internal pressures very well. Moreover, the model can also perform history matching of PDP testing in high accuracy. We found the domain with a larger pore size would have an absolute impact on the apparent permeability. The variables which can influence domain pore size, such as compressibility, effective stress, Biot's coefficient, etc., will be directly related to the apparent permeability of the shale. The mass-exchange-rate coefficient can dominate the gas transport between two domains, deciding the final constant pressure in the PDP testing. The fitting data from this modified dual-porosity-permeability model were validated by two different types of measuring experiments. The model is confirmed and can represent shale gas transport correctly. The research outcome can benefit the optimization of gas-field designs and hydraulic fracturing in horizontal wells in unconventional shale reservoirs.

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Pore-scale CFD based estimation of permeability decline in porous media due to fines migration

Authors: Pramod Bhuvankar[1]; Abdullah Cihan[1]; Jens Birkholzer[1]

[1] *Lawrence Berkeley National Laboratory*

Corresponding Authors: jtbirkholzer@lbl.gov, acihan@lbl.gov, pbhuvankar@lbl.gov

Migration of fine particles in porous media is of interest to oil recovery, geothermal energy, and geological CO2 storage [1,2,3] applications. In fluid injection applications such geological porous media, the clay fines detach due to sharply decreasing salt concentrations near the low-salinity fluid injection wells, migrate, and finally clog the pores, which leads to an increase in hydraulic resistance in porous media [4]. This phenomenon of permeability decline is known to reduce the well injectivity. Efforts to mitigate this problem will require an understanding of the behavior of fines in porous media. In the current work we use computational fluid dynamics to understand the permeability impairment caused by mobile clays clogging the pores. We model the clay fines and the grains as immersed solids using the immersed boundary method coupled with a finite-volume based solver.
We use a 2D finite-volume based Navier-Stokes solver for our simulations. To simulate the flow around mobile and stationary solids we employ the immersed boundary method developed by Bigot et al. 5. The computational domain is composed of 'liquid'and 'solid'regions. We solve the following equations for the incompressible momentum transport in the said regions:
$\nabla.u = 0$
$\rho\left(\frac{\partial u_i}{\partial t} + u_j\partial_j u_i\right) = -\frac{\partial P}{\partial x_i} + \mu\partial_j\partial_j u_i + \rho g_i + f$
Here, f is a force added to ensure that the solid region obeys rigid body motion. A control volume analysis around the solid region results in the following equations for the linear and angular momenta of the clays:
$\frac{\partial u_p}{\partial t} = g - \frac{1}{(\rho_p-\rho)V_p}\int_{V_p}\rho f dv$
$I_p\frac{\partial \omega_p}{\partial t} = -\frac{\rho_p}{(\rho_p-\rho)V_p}\int_{V_p}\rho r\mathrm{x} f dv$
The velocity and angular velocity of the solid are imposed in the solid region. The solid-liquid interface is modeled using the level-set formulation where the interface is represented by the zero level of the distance function. Collisions between the mobile clay particles and the grains are modeled by using a spring-damper model that is activated when the distance between any two solid bodies is below one cell width.
We consider a 2D computational domain comprising of an idealized random porous medium with an average grain size of 20μm. The clay particles are considered to be circular in shape and have a

mean diameter of 3.5μm. The computational domain has periodic boundary conditions along X and Y directions with a length of 80μm along each direction. A pressure gradient is applied to cause a flow through the porous medium and we simulate the movements of the fines along with the fluid flow in the domain.
We observe from our simulations that the fines become trapped in the narrow pore spaces altering the path of the fluid. We also observe bridging structures when multiple particles compete for the same pore space. For a porous medium with 57% porosity and a clay concentration of $0.05g/cm^3$, we observe an 83% decline in permeability as a result of the pore clogging. Our new pore scale model will be used to determine the macroscopic relationships between the permeability decline and the concentration of the released fines from grain surfaces and the captured particles in pore throats in realistic porous media.

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Nanoscale contact angle characterization of a water/oil/calcite system using atomic force microscopy

Author: George Savulescu[1]

Co-authors: Maja Ruecker [1]; Alessio Scanziani [1]; Apostolos Georgiadis [2]; Paul F Luckham [1]

[1] *Imperial College London*

[2] *Shell Global Solutions International B.V.*

Corresponding Authors: p.luckham01@imperial.ac.uk, alessio.scanziani16@imperial.ac.uk, m.rucker15@imperial.ac.uk, a.georgiadis@shell.com, george.savulescu16@imperial.ac.uk

Wetting is a parameter controlling multiphase flow behaviour in porous media and therewith is of crucial importance for a wide range of applications including oil-recovery. Often, micro-computed tomography is used to assess the wetting behaviour of oil/brine/rock systems reflecting a reservoir through in-situ contact angle measurements [1,2]. However, recent studies demonstrated that

sub-resolution nano-scale characteristics of the internal surface of the porous rock, facilitate the formation of thin water films, which influence the flow behaviour and wetting response as well as potential wetting alteration [3,4,5,6]. Atomic force microscopy (AFM) could be utilized as an alternative technique to characterise the internal surface of porous rock and nano-scale fluid films within it [5,6].
This study starts from an AFM-imaged model oil-brine-calcite system, which manifests in form of water-droplets along the solid surface with a roughness R < 20 nm. We analysed the main interface parameters, such as contact angle distributions and 2-phase interfacial areas, and the droplet volumes. The data demonstrates a relationship between the volume and surface areas, which deviates from a perfect spherical cap model, reflecting homogenous wetting and indicates pinning effects. Pinning and depinning has been shown to have important consequences on displacement patterns in multiphase flow in porous media [7]. The measured contact angles are found to be quasi-symmetrically distributed in a range between 10° and 30°. The average contact angle values display slight variations for each droplet. When assessing the locations at which the contact angles were measured individually, the variation was found to follow structural characteristics of the investigated surface. We anticipate this essay to be a starting point for investigations of roughness effects of the internal rock surface on multiphase flow behaviour at the nanoscale using AFM.

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Effect of soil saturation on the stability of soil slopes during rainfall infiltration

Authors: Paiman Shafabakhsh[None]; Marwan Fahs[1]; Renaud Toussaint[2]

[1] *ENGEES-LHYGES*

[2] *IPGS, CNRS, Univ. Strasbourg & PoreLab, Univ. Oslo*

Corresponding Authors: fahs@unistra.fr, paiman.shafabakhsh@student.sharif.edu, renaud.toussaint@unistra.fr

The soil stability is of a prime important hydro-mechanical problem in the aspect of natural risk management. Slope instabilities and landslides are commonly associated with events of intense rainfall. Changes in soil saturation cause changes in suction forces in the deformable porous medium. This problem is often investigated using the equilibrium state via the local factor of safety method. Based on the equilibrium state, this method allows for evaluating a local safety factor that can represent the risk of landslide. The local safety factor is usually calculated numerically. The intense rainfall increases the soil saturation and in consequence the load. The unsaturated flow and the change in soil saturation are often modeled with the Richard's equation. This equation is coupled to the mechanical momentum balance equation representing the static equilibrium and the linear elasticity model as constitutive relation. The existing models neglect the effect of saturation on the soil properties. However, it is clear that, the risk of landslide can be significantly affected by the processes of capillary surface tension. Thus, it is important to include these processes in modeling studies. In this work, we suggest a new mathematical model, at Darcy's scale, for the investigation the stability of soil slopes during rainfall infiltration. The new model can effectively consider the capillary surface tension surface forces which are derived by an up-scaling procedure. The new mathematical model is solved using the finite element method via COMSOL Multi-Physics. Several benchmarks are simulated to validate the developed numerical model. The validated model is then used to investigate a hypothetical case of soil slopes. Comparison between the standard model (neglecting the surface tension effects) and the new developed model (taking into account the surface tension forces) is performed. It is found that considering the surface tension forces leads to an increase in the magnitude of stress tensors over the domain, and consequently, we would have a higher risk of landslide. A detailed parameter sensitivity analysis of the new developed model is performed to understand effect of pertinent parameters on the local safety factor.

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Residual-driven online Generalized Multiscale Finite Element Method for the poroelasticity problem in fractured and heterogeneous media

Author: Aleksei Tyrylgin[1]

Co-authors: Maria Vasilyeva ; Eric T. Chung [2]; Yalchin Efendiev [3]

[1] *Multiscale model reduction Laboratory, North-Eastern Federal University:*

[2] *Department of Mathematics, The Chinese University of Hong Kong (CUHK), Hong Kong SAR*

[3] *Texas A&M, USA*

Corresponding Authors: efendiev@math.tamu.edu, koc9tk@mail.ru, vasilyevadotmdotv@gmail.com, eric.t.chung@gmail.com

We consider the poroelasticity problem in fractured and heterogeneous media. The mathematical model contains a coupled system of equations for pressures and displacements. We present a coarse grid approximation based on the Generalized Multiscale Finite Element Method (GMsFEM). The GMsFEM consists of offline and online stages. In the offline stage, we construct multiscale basis functions based on the solution of local spectral problems defined in the snapshot space for pressure and displacements. Then, we enrich the offline multiscale space by additional online coupled multiscale basis functions. We present numerical results for poroelasticity problems in fractured and heterogeneous media.

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Modeling wood shrinkage during pyrolysis : a major challenge for second generation biofuels.

Authors: Jean Lachaud[None]; Michael Meyer[1]; Cyrille Metayer[1]; Marin Virey[2]; Wahbi Jomaa[2]; Jérémy Meurisse[3]

[1] *University of New Caledonia*

[2] *University of Bordeaux*

[3] *NASA Ames Research Center*

Corresponding Author: jean.lachaud@u-bordeaux.fr

Biomass conversion techniques can be split into three main routes: biochemical, physicochemical, and thermochemical. Biochemical conversions include digestion either anaerobic (biogas production) or aerobic (compost) and fermentation that produces sugars and then ethanol with the help of yeast. The physico-chemical conversion is the production of vegetable oil by physical and/or solvent extraction. Finally, the thermochemical conversions regroup pyrolysis (production of char and bio-oil), combustion (production of heat), an gasification (production of a combustible gas) [Jeanmart2019]. Pyrolysis allows converting second generation biomass - that is, non-food biomass in general and wood in particular. During the pyrolysis process wood releases bio-fuel and loses about 50% of its mass and volume. The solid residue is a pure carbon char. The overall geometrical shrinkage and the intrinsic microstructural evolutions strongly impact heat and mass transfer. Heating rate and pyrolysis gas transport within the pores of wood are key phenomena in the conversion process, not only affecting the rate of production but also the nature of the molecules that are produced [Lachaud2017]. Understanding and modeling shrinkage in combination with the physico-chemical phenomena is critical for the development of the field. To date, simplified mono-dimensional "spring" models have been used. This work presents the first three-dimensional linear elasticity model fully coupled to a volume-averaged heat and mass transfer and pyrolysis model. The model has been implemented in the Porous material Analysis Toolbox based on OpenFoam, released Open Source by NASA (www.pato.ac) [Lachaud2014]. The tool has been used to analyze pyrolysis experiments carried out at 600℃ on pine wood cylinders (diameter : 19 mm, length : 30 mm). A satisfactory preliminary agreement is obtained both on internal thermocouple measurements as a function of time and on the prediction of the final shape. It is shown that when accounting for shrinkage the accepted material properties, such as char conductivity, are no longer correct. This is not a surprise as they were historically tweaked to encompass shrinkage effects.

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Transition from micro-scale to macro-scale modeling of solute transport in drying porous media

Authors: Faeez Ahmad[None]; Rahimi Arman[1]; Evangelos Tsotsas [2]; Marc Prat[None]; Abdolreza Kharaghani[3]

[1] *Thermal Process Engineering, Otto von Guericke University Magdeburg*

[2] *Thermal Process Engineering, Otto von Guericke University Magdeburg, Germany*

[3] *Otto von Guericke University*

Corresponding Authors: mprat@imft.fr, abdolreza.kharaghani@ovgu.de, faeez.ahmad@ovgu.de, evangelos.tsotsas@ovgu.de

Drying of capillary porous media initially saturated with saline water 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 are still questionable at this stage. In this work, we solve the classical advection-diffusion equation for solute transport in an isothermally drying capillary porous medium for the limiting condition of capillary-dominated regime. The solution of the continuum model is compared with pore network simulations. The results of both models are analyzed in terms of local solute concentration profiles for different values of network saturation. On this basis, the ability of the continuum model to reciprocate the pore network results is assessed. In order to improve the prediction capacity of the continuum model for solute transport, the degree of heterogeneity in the liquid phase structure is characterized by performing pore network Monte-Carlo simulations. Based on the statistical analysis of Monte-Carlo simulations, we compute the probability of first solid crystals to appear in the respective liquid phase elements. We observe that 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.

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Global scale prediction of long-term variations of soil salinity and sodicity

Authors: Amirhossein Hassani[1]; Adisa Azapagic[2]; Nima Shokri[1]

[1] *The University of Manchester*

[2] *Department of Chemical Engineering and Analytical Science, The University of Manchester*

Corresponding Authors: nima.shokri@tuhh.de, amirhossein.hassani@manchester.ac.uk

Soil salinization is among the major threats affecting the soil fertility and stability. An accurate estimation of the severity and spatial distribution of the salt-affected land is central to our understanding of the naturally occurring or human-induced land degradation processes related to salinization. To a great extent, current studies on the long-term variability of soil salinity are limited to regional-scale analysis and when it comes to large-scale mapping, a globally consistent analysis of the various aspects of salt-affected soils'dynamics is rare. Here, we quantify the different facets of variability in the salinity and sodicity levels of the top 30 cm soil layer at the global scale for the period 1980-2018 at a ~1 km spatial resolution. This is realized by developing two-part machine learning-based predictive models of the soil EC¬e (electrical conductivity of a saturated soil paste extract) and ESP (exchangeable sodium percentage). These models predict ECe and ESP as target variables at different times, locations, and depths, based on predictors'values. Meaningful descriptive statistics of

variability in ECe and ESP predictions were then derived and used to generate a set of univariate thematic maps, quantifying the different facets of soil salinity and sodicity variation over the past four decades. Among 43 predictors, soil classes, depth from the surface, Fraction of Absorbed Photosynthetically Active Radiation (FAPAR), and temperature of different soil layers were found to be the most significant predictors for prediction of the target variables. Our analysis reveals that the total area of salt-affected soils has been geographically highly variable, showing both decreasing and increasing trends at the country to continental scales. These findings and the provided global scale datasets inform land and water resources management strategies, help tracking the recent hotspots of the soil salinization, and can be used as a forcing parameter in predictive models of crop's growth simulation.

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Scale-dependence of Reaction Rates in Porous Media and Physical & Chemical Heterogeneity

Authors: Branko Bijeljic[1]; Thomas David Serafini de Oliveira[2]; Yousef Al-Khulaifi[None]; Qingyang Lin[2]; Martin Blunt[2]

[1] *Imperial College*

[2] *Imperial College London*

Corresponding Authors: b.bijeljic@imperial.ac.uk, q.lin11@imperial.ac.uk, m.blunt@imperial.ac.uk, thomas.oliveira@centraliens.net

Reactive transport of solutes in porous media is encountered in many applications, such as contaminant transport and remediation in subsurface, acidization to enhance permeability in oil recovery, and packed bed reactors in chemical engineering. A principal outstanding problem in subsurface reactive transport is to determine the effective reaction rates from the pore-scale upwards. This is of key importance in highly heterogeneous natural porous media such as carbonate rock. Carbonates are known to have a significant portion of their pore space as micro-porosity, which may lead to a very wide distribution of local velocities, increasing transport heterogeneity that affects mixing and ultimately reaction. Hence, there is a need for a systematic methodology that can identify and quantify the impact of physical and chemical heterogeneity on the reaction rates. Moreover, in many problems additional complexities arising from coupling of multispecies transport and reaction reversibility need to be accurately addressed.

We develop a new methodology termed Screening Pore-Scale Imaging and Modelling (SPIM) that can be used to predict the fluid/solid reaction rates based on the systematic characterization of both physical and chemical heterogeneity in multi-mineral systems [1-3]. Physical heterogeneity of the rocks is classified in accordance with the velocity distributions obtained by numerical flow simulation on dry micro-CT images. Spatial distribution of chemical heterogeneity is also provided from the images. Performing and analyzing coreflooding CO2/brine/carbonate experiments, we show that mineral reaction rates are an order of magnitude lower than the corresponding batch rates due to mass transfer limitations. We introduce a new metrics quantifying coupled reactive transport behaviour, which describes proximity of reacted minerals to the fast channels and slow regions. Overall, a higher degree of physical (initial pore structure and associated velocity field) and/or chemical (intrinsic reaction rates and mineral distribution) heterogeneity promotes the preferential channelling effect, as opposed to uniform dissolution.

Furthermore, we simulate 3D multispecies fluid/fluid reversible reactive transport [4] in a micro-CT image of carbonate rock that entails spatially resolved information on connected micro-porosity.

Direct numerical simulation of Darcy-Brinkman 5 and advection-diffusion transport equations are coupled to a general geochemical model [6]. We demonstrate salient features of mixing and reaction arising as a result of intricate pore space heterogeneity. We show that evolution of rates of formation and consumption is species-dependent, and highly distinct in macro- and micro-porosity. Well-mixed regions result in asymptotic reaction rates. In contrast, incomplete mixing leads to transient and, for some species, even non-monotonic reaction rate behaviour.

Overall, we conclude that reactive behaviour is simultaneously influenced by pore space heterogeneity, multispecies reactive transport, and reaction reversibility. This means that for complex reversible reactions in heterogeneous porous media, species-specific behaviour needs to be examined for an accurate determination of reaction rates.

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A posteriori error estimates and adaptive solvers for porous media flows

Author: Martin Vohralik[1]

[1] *Inria Paris*

Corresponding Author: martin.vohralik@inria.fr

Numerical simulation of porous media flows is a domain of permanently increasing importance. But can we assess how large is the error between the predicted numerical result and the unknown solution? And could the same precision be achieved faster? I will present some answers to these questions for several model porous media flow problems, starting from the steady linear single-phase Darcy flow, passing through problems involving reaction, advection, nonlinearities, degeneracies, or thermal effects, and ending with multi-phase multi-compositional flows with phase change. Guaranteed and fully computable bounds are obtained for the simpler problems, both for error in some

energy norm or for error in a quantity of interest. A unified framework covering common discretization schemes (finite elements, finite volumes, discontinuous Galerkin) is presented, general polygonal/polyhedral meshes are discussed, and cheap implementations of the estimates are addressed. For all models, different error components are distinguished such as space discretization, time discretization, linearization, or algebraic. Then adaptive stopping and balancing criteria are designed which allow to invest the computational effort where needed and considerably speed-up simulations for the given relative precision target.

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Asymptotic analysis of immiscible two-phase flow with moving contact line in a thin strip

Authors: Carina Bringedal[1]; Iuliu Sorin Pop[2]; Stephan Lunowa[3]

[1] *University of Stuttgart*

[2] *Hasselt University*

[3] *Hasselt University, Computational Mathematics (CMAT)*

Corresponding Authors: carina.bringedal@iws.uni-stuttgart.de, stephan.lunowa@uhasselt.be, sorin.pop@uhasselt.be

We consider a model for the flow of two immiscible fluids in a two-dimensional thin strip of varying width. This represents an idealization of a pore in a porous medium. The interface separating the fluids forms a freely moving interface in contact with the wall and is driven by the fluid flow and surface tension. The contact line model incorporates Navier slip boundary conditions and a dynamic and possibly hysteretic contact angle law.
We assume a scale separation $\varepsilon \ll 1$ between the typical width and the length of the thin strip. Based on asymptotic expansions and letting ε approach zero, we derive effective models for the two-phase flow. These models form a system of differential algebraic equations for the interface position and the total flux. The result is a Darcy-type equation for the flow, combined with a capillary pressure - saturation relationship involving dynamic effects.
Finally, we provide some numerical examples to show the effect of a varying wall width, of the viscosity ratio, of the slip boundary condition as well as of having a dynamic contact angle law.

Keywords:
Asymptotic expansions;
Two-phase flow;
Freely moving interface:
Dynamic contact angle;
Thin strip;
Upscaled models

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Pore-Scale Direct Numerical Simulation of Flow and Transport in Porous Media

Author: Qinjun Kang[1]

[1] *Los Alamos National Laboratory*

Corresponding Author: qkang@lanl.gov

Flow and transport processes in porous media are pervasive in energy and environment. A better understanding of these processes is critical for addressing important problems such as petroleum and geothermal energy production, geological storage of CO2 and nuclear waste, as well as optimization of energy storage and conversion devices for improved performance and durability. With the rapid advancement of computers and computational methods, and rapid development of X-ray tomographic imaging techniques, pore-scale direct numerical simulation (DNS) has become an increasingly important tool to analyze the underlying physical, chemical, and biological processes involved in flow and transport in porous media, to develop the microstructure-transport property relationships, and to derive the constitutive parameters for larger-scale modeling. In this talk, I will present our recent work on pore-scale DNS of various flow and transport phenomena, including supercritical CO2 displacing brine in a heterogeneous micromodel and real rock; two-phase flow in heterogeneously wet porous media and fractures; corrosion/oxidation of uranium dioxide under repository/reactor conditions; as well as pore-ionomer interfacial reactive transport processes in proton exchange membrane fuel cell catalyst layers. I will also present some of our ongoing work using machine learning to develop emulators for pore scale models and to bridge different scales.

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Designing porous materials for improved fuel cell and electrolyzer performance

Author: Aimy Bazylak[1]

[1] *University of Toronto*

Corresponding Author: abazylak@mie.utoronto.ca

The polymer electrolyte membrane (PEM) fuel cell and electrolyzer are composed of multiple porous materials, including the catalyst layer, microporous layer, and substrate. Commercial materials, whether by design or not, typically exhibit highly heterogeneous material and chemical properties. In order to reach cost targets for widespread commercial adoption, we must realize materials that enable more effective multiphase flow phenomena than what currently exists. Mass transport losses in PEM fuel cells and electrolyzers are both prohibitively significant. However, designing these materials requires the a priori knowledge of how the heterogeneous properties of the porous materials and their interfacial contacts influence electrochemical performance. In this work, I will discuss these critical design factors (heterogeneous porous materials and nature of interfacial contacts) and how they influence the flow and mass transport behaviour in PEM fuel cells and electrolyzers. I will also discuss the new materials we have designed and fabricated, informed by in-house numerical modelling and tested through a combination of in operando and ex situ X-ray and neutron beam characterization approaches.

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Addressing the water scarcity problem with thermal osmosis

Author: Signe Kjelstrup[1]

[1] *Norwegian University of Science and Technology, NTNU, Trondheim*

Corresponding Author: signe.kjelstrup@ntnu.no

To describe flow in porous media Darcy's law has been central, and rightly so. The pressure difference, or more generally the chemical potential difference, is a major driving force of flow. Other driving forces for transport, electric and gravitational fields for instance, have more particular applications. Less is known on thermal driving forces for transport in porous media. On the other hand, not only industry, also nature provide large amounts of waste heat. The use of this heat to do useful work, is therefore of interest, theoretically as well as practically.
In this lecture, I will examine the theoretical and practical conditions for a particularly important case of two-phase flow in porous media; namely the flow of water using vapor-gap membranes and a waste heat source to provide a driving force. The phenomenon is called thermal osmosis. In thermal osmosis, heat can be used to clean water and drive a turbine, as well. In nature, the phenomenon can be related to frost heave.
There is a world - wide scarcity of clean water, and the United Nations have declared that the decade 2018-2028 be used to "Avert a global water crisis". In this contribution to help avert the problem, we shall see that the theoretical basis of non-equilibrium thermodynamics can help understand the mechanism of thermal osmosis. An exact description can then follow and lend itself to experimental control and optimization. Other applications are close at hand.

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Microscopical lesions of the transport system of organs and their relation to clinically observable large-scale phenomena

Author: Dominik Obrist[1]

[1] *University of Bern*

Corresponding Author: dominik.obrist@artorg.unibe.ch

Many diseases are directly related to microscopical lesions of the transport system of organs: Cystic fibrosis, for example, leads to obstructions of the smallest airways; Multiple sclerosis can be

connected to leaking capillaries in the brain; and recovery after a heart attack can be limited by microvascular obstruction of the heart muscle. Reliable and accurate diagnosis of such lesions is important for the early detection and targeted treatment of the diseases. Unfortunately, their clinical diagnosis is very difficult, because the small structures are inaccessible to interventional instruments and the resolution of imaging modalities is too coarse. Therefore, diagnosis is typically based on limited information obtained from large-scale phenomena which can be observed clinically.

We developed multi-scale models which allow us to infer the state of microscopical lesions from observable large-scale phenomena. To this end, it is helpful to model the smallest structures of an organ as porous medium which is coupled with a large-scale advective transport model. We will present several computational and experimental multi-scale models of organs and demonstrate how they can be used to support the diagnosis of diseases of the brain, heart and lung.

Diagnosis of lesions of microvascular structures in the human body is difficult, because these structures are inaccessible to classical interventional instruments and the resolution of clinical imaging modalities is too coarse.

Many organs of the human body can be split into large scale systems and small scale systems. Whereas the large scales are typically connected to transport processes (e.g. arteries transporting blood from the heart to the tissue), the small-scale systems are seen as the place for substance exchange (e.g. capillary blood vessels where o2 and CO2 are exchanged between blood and tissue).

Pathologies of the small scale structures are difficult to diagnose and treat because of a lack of accessibility of these structures with clinical instruments and a lack of observability with the available imaging modalities. Therefore, there is a need for developing diagnostic methods which allow us to infer pathological conditions at small scale from observations at large scale.

I will present methods on the example of three different organs: diagnosis of microvascular lesions in the myocardium after heart attack, in the brain of MS patients and in the lung for Cystic fibrosis and congenital microvascular malformations in the extremities.

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Topology and its effects on fluid flow

Author: James McClure[1]

[1] *Virginia Tech*

Corresponding Author: mcclurej@vt.edu

Geometric structure plays an essential role in many transport processes. Within this context, topology provides a way to measure how material is connected within a system. In a multiphase flow, topological changes occur due to coalescence and snap-off events that fundamentally alter the fluid structure and behavior. These changes can be understood quantitatively based on geometric invariants, which include the Euler characteristic as a topological measure. This talk will consider topological changes in the context of geometric evolution. Geometric laws that constrain the possible shapes that an object can attain will be used to infer the relationship between geometric invariants. Noting that changes to the toplogy of an object occur as discrete events, the fundamental mechanisms that drive these changes will be considered in detail. The associated physical consequences will be examined from the molecular scale, the pore-scale, and the reservoir scale.

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Porous Media, Small and Large: From Atomistic Modeling of Nano-Porous Membranes to Modeling of Flow and Transport in Geological Formations

Author: Muhammad Sahimi[1]

[1] *University of Southern California*

Corresponding Author: moe@usc.edu

Flow, transport, reaction, adsorption and deformation (FTRAD) constitute a fascinating set of phenomena that occur in a wide variety of porous media and materials over widely disparate length scales, from molecular, to pore, core, and field scales.

In this presentation four classes of fundamental problems are described and the approaches to their modeling are discussed. We first describe a process-based modeling of fabrication of a nano-porous membrane based on quantum mechanical calculations and molecular dynamics simulations. We then outline a general approach to modeling of adsorption and swelling of several types of core-scale porous materials. Next, the problem of reconstruction of porous materials and media based on limited data, such as their two- or three-dimensional images is described, and a new method based on curvelet transforms for speeding up simulation of the FTRAD in such images is discussed. Finally, the problem of upscaling from core to field scale is described and a multiresolution approach to the problem based on wavelet transformations is
discussed.

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Modelling the behaviour of skin after deep tissue injury using poro- and morpho-elastic models

Author: Fred Vermolen[1]

[1] *Delft University of Technology*

Corresponding Author: f.j.vermolen@tudelft.nl

More than 12 million people per year get seriously injured as a result of burn accidents. About one million people per year die as a result of the consequences. Serious skin trauma is often accompanied with heavy scar formation and with the formation of contractures, which refer to skin contractions that are so severe that the patient is faced with disability.

In order to improve the quality of life of patients, it is important to investigate the biological mechanisms behind the evolution of skin. Investigation of skin is done by clinical and in-vitro experiments, and by the formulation of hypotheses. To match theory to experiments, which come in as patterns and numbers, quantification of the developed theory is crucially important. Therefore, mathematical models help develop insight into the behaviour of skin after skin trauma.

Skin mechanics is an important aspect of the formation of contraction. One of the important features is that deformations are plastic. In this talk, a morpho-elastic model will be presented, as well as the underlying mathematical and numerical issues to simulate skin mechanics. Furthermore, some results from poro-elasticity will be discussed.

Since there are large patient-to-patient variations, uncertainty is an important aspect. In the talk, uncertainty aspects will also be dealt with using stochastic (partial) differential equations and stochastic processes.

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Multi-scale in-situ fluid monitoring to understand and model multiphase flow in porous media

Author: Olga Vizika Kavvadias[1]

[1] *Institut Francais du Petrole Energies nouvelles (IFPEN), France*

Corresponding Author: olga.vizika-kavvadias@ifpen.fr

Transport phenomena in porous media are encountered in many situations of practical and scientific interest, where determination of transport properties remains a challenging issue. They may concern natural porous media, such as soils, aquifers or hydrocarbon reservoirs, or artificial ones, such as filters, fuel cells, catalysts and concrete.

Multiphase flow in natural porous media is essential in a wide range of phenomena and applications in geosciences, including hydrocarbon formation and migration, oil and gas production, enhanced oil recovery, underground energy or CO2 storage, water resources management or soil remediation. Understanding and predicting fluid displacement mechanisms at the relevant scale is one of the big challenges in basin and reservoir modeling.

The description of the transport of fluids in geological formations relies upon advances on the characterization and modeling of natural systems in a large spectrum of time and length scales. The complexity of transport processes in these systems is due to the natural complexity and heterogeneity of geological structures as well as to the dynamics of the multiphase fluid displacement and its coupling with mechanical, thermal, chemical and biological processes.

Information on the pore space geometry and topology and on fluid displacement is essential to understanding of mechanisms and modeling. In 2D, micromodel experiments and advances in microfluidics bring qualitative and quantitative information on the motion of fluid/fluid interfaces in model

systems down to the micron scale. In 3D, X-Ray 3D-imaging has proved to be a key technology to study multiphase flow in porous media with a continuous quest for space and time resolution.

Experimental observation has to be intimately linked to pertinent theoretical modeling taking into account the relevant physics of the studied phenomena at the right scale. Advances in molecular dynamics, lattice-Boltzmann or pore-network modeling methods combined to upscaling considerations permit to simulate complex flow regimes and to run laboratory and numerical experiments on comparable sample volumes.

Through selected examples, on the combination of experimental observation and theoretical analysis at different scales, we demonstrate the necessity of adapting space and time scale to the studied phenomenon, and the complementarity of different methods to investigate multiphase flow in porous media.

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Electrokinetic and ion transport in micro/nanoporous media

Author: Moran Wang[1]

[1] *Tsinghua University*

Corresponding Author: mrwang@tsinghua.edu.cn

Ion transport is ubiquitous in aqueous environments in biological, geological, chemical and environmental systems. Electrokinetics plays a very important and key role in some special cases where pore size is comparable to the screening length of electrical double layer. The applications include tight oil/gas exploration and development, radiative waste disposal, high-quality water purification, and even ion channels in cells. This talk will present (1) electrokinetic and interface theories for ion transport in micro/nanoporous media; (2) a mesoscopic numerical framework for predictions and the validations by comparisons with theories and experimental data; (3) multiscale analysis in both spacial and temporal scales for special applications.

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Coupling free flow and porous-media flow, and its applications to aerospace and mechanical engineering

Author: Guang Yang[1]

[1] *Institute of Refrigeration and Cryogenics, Shanghai Jiao Tong University*

Corresponding Author: y_g@sjtu.edu.cn

The coupling of free flow and porous media flow is extensively involved in technical, environmental, and biological systems. In the first part of the talk, I will present the fundamental research with respect to the momentum transfer characteristics at the coupling interface. Then in the second part, I will talk about the roles of this coupling effect in three specific applications from the field of aerospace and mechanical engineering, namely vapor chamber heat-transfer system, transpiration cooling technology, and propellant acquisition device. The coupled free/porous media flows have also found to be often indivisible with turbulence, heat transfer, and phase change. Progress of the parameter optimization studies conducted by our group for the above mentioned applications will also be presented.

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HydroGrid: Emerging Technologies for Global Water Quality and Sustainability

Author: Lilit Yeghiazarian[1]

[1] *University of Cincinnati*

Corresponding Author: yeghialt@ucmail.uc.edu

Water problems cannot be solved piece-meal, one issue at a time. Rather, a holistic, systems-based approach is needed to manage the global water system sustainably. This talk will introduce the concept of the HydroGrid as a framework to describe connected water systems that encompass surface water and groundwater, the natural environment and built infrastructure. Drawing upon the knowledge and engineering experience employed in electrical grid operations, we outline mirroring concepts in the HydroGrid, with a particular focus on monitoring, analysis, and control of water quality.

We will discuss emerging technologies in advanced materials, porous media design and modeling, signal transduction and wireless communications that enable development of autonomous mobile devices for dynamic water quality monitoring. As this technology matures, the devices will have the capability to stream real-time or near-real-time data for analysis with stochastic models of contaminant fate and transport. Modeling results, combined with controllability analysis of water systems, can then be used to determine system-wide prevention and mitigation strategies. Progress is measured with probability-based metrics of HydroGrid sustainability such as reliability, vulnerability, and resilience.

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Contact line motion using the Volume of Fluid method

Author: Stéphane Zaleski[1]

[1] *Institut Jean Le Rond d'Alembert*

Corresponding Author: stephane.zaleski@gmail.com

Wettability, contact line dynamics and surface tension are essential in the pore scale motion of interfaces. Since it is difficult to resolve numerically the small interface thickness a sharp interface model seems the only practical solution. However in the context of this sharp interface model Huh and Scriven wrote "not even Herakles could sink a solid if the physical model were entirely valid". The resolution of this paradox has occupied a large number of investigators, however a popular fix is to assume a Navier boundary condition for the tangential fluid velocity on the solid surface, which introduces a slip length l. We discuss the performance of such slip length models in various regimes. The sharp interface model is implemented using a Volume Of Fluid (VOF) method in the context of several free codes developed at d'Alembert Institute of Sorbonne Université and the FLOW lab at KTH. The results are compared to experiments and molecular dynamic simulations.

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