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Book of Abstracts

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4

Analysis and Optimization of Main Controlling Factors Affecting Oil Recovery of Sandstone Reservoirs After Long-term Waterflooding

Author: Shanglin Liu[1]

Co-authors: Anzhu Xu [1]; Jincai Wang [1]; Jun Ni [1]; Lun Zhao [1]; Shujun Han [1]; Xuanran Li [1]

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The waterflooding development performance of sandstone reservoir is affected by several geology and engineering factors. This research investigates the effects of reservoir heterogeneity, oil viscosity, water injection intensity and well spacing on sandstone reservoir waterflooding development, considering the changes of reservoir physical properties after long-term waterflooding by applying time-varying numerical simulations. By factor normalization and multiple regression methods, the relationship between recovery factors and four main controling factors is established, and the weight coefficients of each parameter are obtained, the optimal injection-production parameters are further determined under different reservoir conditions. This study has certain guiding significance for the evaluation of waterflooding development and the production optimization of sandstone reservoir.

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MS15 / **5**

A deep learning enabled massive parallel simulator for porous media flow

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Due to the complex composition of oil and gas resources, reservoir engineers usually switch between different mathematical models when describing the properties of petroleum reservoirs. In addition to the commonly used black oil model, various compositional models have been proposed. Some EOR techniques, such as polymer flooding, must be simulated based on the framework of compositional models. Some other applications of porous media flow, such as CO2 sequestration, groundwater contamination, and geothermal resource development, can also be simulated using compositional models. But the compositional models tend to be associated with more complex PDEs, more variables, and higher computational costs. In this talk, we will discuss a general-purpose compositional framework and our efforts in developing its solution methods, including discretizations, nonlinear solvers, linear solvers, parallelization and AI capabilities. Furthermore, we will introduce an open-source software project for simulating multi-component multi-phase porous media flow.

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MS08 / **6**

Dispersion and Straining Behaviors of Non-Spherical Suspended Particles in Saturated Randomly Packed Beads: A Numerical and Theoretical Study

Authors: Yaoming Chen[1]; Dian Fan[2]

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Understanding the transport of particles in porous media, including dispersion and straining, plays a pivotal role in optimizing various engineering processes, such as drug delivery, wastewater treatment, and fracking proppants displacement. While prior numerical endeavors have significantly expanded our understanding of the microscopic behavior of particles within porous media, they have frequently overlooked the shape anisotropy of particles. When particles are non-spherical, such as pills, bacteria, and microplastics, the shape anisotropy of particles may determine their dispersion and straining behaviors in porous media, even in weakly heterogeneous environments like beadpacks.

To bridge this knowledge gap and evaluate our hypothesis, we simulated the Lagrangian transport of 3-D non-spherical particles through a 3-D porous network generated by a randomly sedimented, saturated bead pack, employing a computational fluid dynamics-discrete element method (CFD-DEM) approach. To account for the particles'asphericity as well as its impact on particle transport, we modeled the particles as superquadrics of varying asphericities and implemented a particle-fluid two-way coupling algorithm, where the fluid flow influences particles'motion, and conversely, particles also affect the fluid streamlines.

Our results suggest that, compared to spherical particles, highly aspherical particles tend to migrate along streamlines more readily, resulting in a higher mean dispersivity; such particles also tend to sweep a larger volume of the pore space, leading to a more uniform spatial distribution of retained particles. To support our numerical observations, we report a particle velocity probability distribution function that encompasses the impact of particles'asphericity on their dispersion and straining behaviors. Said function compiles all numerical observations and distinguishes between the straining and dispersion characteristics. We also deliberate on the similarities and differences between this new function and the function applicable to spherical particles, as previously reported [1]. The presented function can be useful in designing particle topology to achieve specific velocity distributions or mean dispersivity of interest.

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MS08 / **7**

Dispersion Control in Fractured Multi-Layer Porous Media System

Author: Bowen Ling[1]

Co-authors: Felipe P. J. de Barros [2]; Runqing Shan [3]

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Multi-layered porous media are present in a variety of natural and engineered systems, and their structure can have a significant impact on flow and transport processes. This study proposes a hybrid analytical-numerical solution to examine the relationship between scalar dynamics and media properties in coupled systems comprising a two-dimensional free flow layer and a heterogeneous porous medium operating under fully developed laminar flow conditions. Perturbation and homogenization methods are used to obtain a set of one-dimensional upscaled equations for passive scalar transport. These equations are then used to develop a semi-analytical solution based on integral transforms, which enables the relationship between the properties of the porous system and scalar mixing and spreading to be determined. To validate the solution for the upscaled system, we compare the results with numerical findings for two-dimensional scalar transport. In addition, we analyze the influence of the multilayered system on macroscopic transport by examining the breakthrough curve, dispersion coefficient, and mixing of the scalar cloud. The results suggest that the semi-analytical solution can be used to optimize and determine the arrangement of porous media properties to achieve desired mixing objectives.

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MS01 / 8

Design of viscosified CO2 for carbon storage in saline aquifers by continuum-scale imaging and modeling

Authors: Abbas Firoozabadi[1]; Boxin Ding[2]

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Carbon capture, utilization, and storage (CCUS) is expected to play an essential role in global decarbonization. Safe and efficient storage of CO2 in saline aquifers requires mobility control to prevent CO2 from exposure and accumulation at the formation top. An effective agent for CO2 mobility control should be carefully tailored with low adsorption in rock surfaces, low injection pressure, and high capacity of carbon storage. Here, we develop and utilize engineered oligomers at very low concentrations to directly viscosify the sc-CO2 and demonstrate their effectiveness for improving CO2 storage in saline aquifers with layered formation. We also present results from X-ray CT imaging to advance the understanding of two-phase CO2-brine flow in layered cores and firmly establish the

transport mechanisms.
X-ray CT imaging of displacement experiments is conducted to quantify the in-situ sc-CO2 saturation spatiotemporally in the brine-saturated porous media with homogeneity and heterogeneity. In neat CO2 injection, the large mobility contrast between the CO2 and brine results in the channeling of CO2 through the high permeability zone, leading to an early breakthrough and low brine production. Direct measurement and in-situ saturation measurement show that there is around 10% difference for cumulative brine production in neat CO2 injection. The difference between the two is attributed to the solubility of the produced water in the produced CO¬2 at atmospheric pressure which has been neglected in the past. We show that when the forgotten effect is accounted for, there is a good agreement between direct measurements and in-situ saturation results. The X-ray imaging demonstrates that the large effect of improved carbon sequestration is attributed to reduction of residual brine saturation from increase in interfacial elasticity from the addition of the oligomers. The combination of mobility control and residual brine saturation reduction is expected to improve CO2 storage in layered formation by effective viscosification at very low concentrations of oligomers. We also develop a model coupled with hydrodynamics and thermodynamics to compare, identify and analyze with the experimental observations from X-ray CT imaging. The model sheds light on understanding the CO2 flow in saline aquifers.

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Poster / 10

Fractal characteristics of natural fractures in continental shale reservoir and their effects on permeability

Author: Xiaoming Wang[1]

Co-author: Junbin Chen [1]

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The development characteristics of natural fractures are restricting the efficient development of low permeability reservoirs, but the existing methods not only cannot achieve a quantitative characterization of natural fractures, also cannot achieve quantitative analysis of their effect on permeability. Therefore, based on fractal theory, SEM technology, image processing and permeability measurement were used to solve this problem in continental shale reservoir. Results show that the development degree of natural fractures varies greatly in different bedding directions, fractal dimension can be used to quantitatively characterize the development degree of natural fractures and reservoir permeability in different bedding directions. Compared with vertical bedding, the fractal dimension of natural fractures in parallel bedding direction is much larger, natural fractures are more developed and have better fractal characteristics. However, the permeability of cores with parallel bedding is much smaller, which is 1/7 of that of cores with vertical bedding. Meanwhile, the permeability of cores with vertical bedding increases with the fractal dimension of natural fractures in vertical bedding direction increasing, while the permeability of cores with parallel bedding decreases with the fractal dimension of natural fractures in parallel bedding direction increasing. The results are of great significance for guiding the efficient development of oil and gas in continental shale reservoir.

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MS06-B / 12

The mathematical model and analysis of the nanoparticle-stabilized foam displacement

Authors: Grigori Chapiro[1]; Pavel Sejas Paz[None]; Tatiana Danelon de Assis[None]

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This work proposes a mathematical model to study the foam displacement in porous media stabilized by nanoparticles [1]. We consider a simplification of the Stochastic Bubble Population balance model in local equilibrium, with nanoparticle dependence inspired by the experimental data from the literature. It consists of a non-strictly hyperbolic system of conservation laws, which is solved for the generic initial and injection conditions. We investigate the existence of a global solution as a sequence of waves following the Conservation Laws Theory and the procedure proposed in [2], where a similar problem was solved for a two-phase flow containing an active tracer (with linear adsorption). When the solution is composed of two or more waves, we present necessary and sufficient conditions to guarantee the compatibility of these wave sequences. The analytical solution for the nanoparticle-stabilized foam displacement in porous media allowed us to quantify the effect of nanoparticles on foam displacement, focusing on the breakthrough time and cumulative water production. In agreement with the literature, when only gas is injected, the breakthrough time and the water production increase with the nanoparticle concentration. Although, we also observe that the effect of nanoparticles is less pronounced for high nanoparticle concentration. Counterintuitively, adding nanoparticles changes the mathematical solution qualitatively, yielding a negligible effect on water production during gas-water co-injection for a certain parameter range. We discuss the most favorable conditions to observe the action of nanoparticles in laboratory experiments.

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MS06-B / 13

Experimental Investigation and Molecular Dynamics Analysis of the Fluid-Fluid Interactions between Binary Surfactant Systems for EOR

Author: Ayomikun Bello[1]

Co-authors: Alexander Rodionov [2]; Alexey Cheremisin [1]; Alina Bazhanova [1]; Anastasia Ivanova [1]

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This work aims to explore the properties and interactions between binary surfactant systems due to their ability to form mixed micelles with lower interfacial tension (IFT). The focus is on determining the synergistic or antagonistic behaviors of these systems for effective application in enhanced oil recovery (EOR) in carbonate oil fields. Our study employed a methodology comprising experimental analysis, mathematical modeling, and molecular dynamics simulations. In the experimental study, we examined eight individual surfactants and six binary surfactant systems at various ratios to determine their critical micelle concentrations (CMCs), using reservoir oil and performing experiments at reservoir conditions. Then, Rubingh's Regular Solution Theory (RST) was applied to evaluate interactions within the binary surfactant mixtures. Finally, using molecular dynamics simulations, we characterized the microscopic interactions to comprehend how hydrophilic and hydrophobic parts of the surfactants interact with surrounding media, and how they self-assemble into aggregates such as micelles or bilayers. The key findings of our work showed that the occurrence of synergism or antagonism in lowering the CMC of binary surfactant mixtures depend on both the concentration of the individual surfactant and the type of surfactant used. Nevertheless, we noted a prevalent synergistic phenomenon in all binary surfactant systems, notably influenced by the concentration of the non-ionic surfactant. Increased concentrations of non-ionic surfactants notably enhanced synergistic interactions, fostering lowered CMC values when combined with anionic, cationic, and zwitterionic surfactants. On the other hand, an excessive concentration of cationic surfactants demonstrated relatively 'weak' synergistic effects, attributed to their comparatively smaller hydrophobic tail. Moreover, the formation of mixed micelles in binary surfactant systems led to a more negative free energy of micellization, thereby achieving synergistic effects between surfactants and resulting in lower CMC values. This emphasizes the crucial role of surfactant concentration in achieving synergistic outcomes within mixed systems. Generally, binary surfactant systems demonstrated lower CMC values compared to single surfactants, suggesting the potential for their use at lower concentrations to achieve desired interfacial and recovery outcomes, thereby reducing operational costs.

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Rock-Fluid Interaction Mechanisms between Binary Surfactants Systems for Enhanced Oil Recovery in a Carbonate Formation

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Carbonate rocks exhibit a complex surface charge, making it challenging to generalize the use of a single surfactant type. Hence, the utilization of binary surfactant mixtures is proposed as a more efficient alternative. This work focuses on static adsorption, wettability alteration, and spontaneous imbibition tests to gain comprehensive insights into the underlying fluid-rock interactions in carbonate formations. The objective is to propose more effective solutions for enhanced oil recovery in carbonate formations. Our study centered on binary surfactant systems and their interactions with carbonate rock. We conducted several laboratory experiments, including static adsorption tests on eight different surfactant systems. This aimed to compare their adsorption behaviors against individual surfactants, with the aim of studying their synergistic interactions. Additionally, wettability and spontaneous imbibition tests were conducted under the reservoir conditions of a producing oil field to understand the primary mechanisms and synergistic effects of binary surfactant systems in enhancing oil recovery from carbonate formations. Our results showed a significant influence of the nonionic surfactant leading a considerable reduction in adsorption values of 53% and 28% in its anionic-nonionic and cationic-nonionic mixtures, respectively. The efficient synergism between binary surfactant systems to reduce surfactant adsorption in carbonate rocks was also confirmed in the physicochemical evaluations with a reduction in both zeta potential and pH values when compared to their individual surfactants. Furthermore, spontaneous imbibition results showed that binary surfactant mixtures exhibit maximum synergism, particularly when they system is composed of of zwitterionic and non-ionic surfactants. This surfactant blend resulted in the highest recovery factor of nearly 60%, signifying significant improvement in oil recovery from carbonate formations. According to the analysis of contact angle, the binary surfactant systems did not significantly change wettability. However, this can be beneficial because it implies that the surfactant molecules are not adsorbed to the rock surface within the porous medium. Instead, they are utilized to their maximum potential within the porous medium. The findings presented in this work demonstrate that careful screening, selection, and combination of binary surfactants can effectively reduce surfactant adsorption, maintain rock wettability, and substantially lower interfacial tension in carbonate rock, ultimately aiming to enhance oil recovery. This approach paves the way for the development of innovative surfactant blends that ensure the economic viability of EOR projects, suitability for CO2 foam sequestration projects, and broad applicability in carbonate formations.

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MS07 / **16**

A robust two-level overlapping preconditioner for Darcy flow in high-contrast porous media

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In this talk, we present a two-level overlapping domain decomposition preconditioner for solving linear algebraic systems obtained from simulating Darcy flow in high-contrast media. Our preconditioner starts at a mixed finite element method for discretizing the partial differential equation by Darcy?s law with the no-flux boundary condition and is then followed by a velocity elimination technique to yield a linear algebraic system with only unknowns of pressure. Then, our main objective is to design a robust and efficient domain decomposition preconditioner for this system, which is accomplished by engineering a multiscale coarse space that is capable of characterizing high-contrast features of the permeability field. A generalized eigenvalue problem is solved in each non-overlapping coarse element in a communication- free manner to form the global solver, which are accompanied by local solvers originated from additive Schwarz methods but with a non-Galerkin discretization to derive the two-level preconditioner. We provide a rigorous analysis indicating that the condition number of the preconditioned system could be bounded above with several assumptions. Extensive numerical experiments with various types of three-dimensional high-contrast models are exhibited. In particular, we study the robustness against the contrast of the media as well as the influences of numbers of eigenfunctions, oversampling sizes, and subdomain partitions on the efficiency of the proposed preconditioner. Besides, strong and weak scalability performances are also examined. The work is partially supported by the Hong Kong RGC General Research Fund (Projects: 14305222 and 14304021).

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MS09 / **17**

Investigate the effect of pore heterogeneity on elastic wave velocity evolution under mineral dissolution process

Authors: Yutian Zhang[None]; Yifan Wu[1]; Fei Jiang[2]; Xiaoguang Wang[1]; Takeshi Tsuji[3]

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Mineral dissolution is a common phenomenon in many subsurface geo-systems, such as carbon sequestration, wastewater disposal and oil and gas recovery. Dissolution can change the topology of porous rock, which affects the rock's geophysical parameters, such as permeability and elastic wave velocity. We numerically investigate the relationships between the evolutions of P-wave and S-wave velocities and permeability induced by mineral dissolution under different pore heterogeneities. We use a linear Boolean model to represent sedimentary rocks with various pore heterogeneities. We reproduce three typical dissolution patterns: compact, uniform and wormhole, by adjusting the Péclet and Damköhler numbers. For these numerical simulations, we use the lattice Boltzmann method to compute the velocity and concentration fields, and the finite element method to compute the strain fields. Our results indicate that the evolution trends of both P-wave and S-wave velocities are similar in all simulations. When the initial pore heterogeneity is fixed, the uniform dissolution pattern cases show a faster decrease of elastic wave velocity as the dissolution progresses; when the dissolution pattern is fixed, the more heterogeneous rock shows a faster decrease of elastic wave velocity. The findings have important implications for subsurface engineering applications involving pore network and fluid path evolutions caused by mineral dissolution.

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Poster / 18

Experimental evaluation of dynamic seepage in tight/shale reservoirs under the coupling of matrix fractures based on NMR

Author: Meng Du[None]

Co-authors: Shuyi Lu ; Zhengming Yang ; Weifeng Lyu ; Xinliang Chen ; Xiang Qi ; Pengwei Fang ; Zhuoying Dou

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The imbibition and displacement between fractures and matrix have a significant effect on the development of tight/shale reservoirs, a combination of dynamic displacement and imbibition online physical simulation method was established by integrating nuclear magnetic resonance (NMR) and CT scanning. Through real-time dynamic monitoring of multiphase flow and migration behavior of crude oil in each stage of dynamic imbibition, the development effect of dynamic imbibition and the micro-production mechanism of pore throats with different sizes of tight/shale oil were quantitatively studied. The effects of displacement pressure, permeability, and fractures on the dynamic

imbibition effect and pore crude oil production were analyzed. On this basis, the dynamic seepage process of fracking-soaking-backflow-production integration was simulated, which reveals the dynamic production characteristics of different development stages and their contribution to enhancing oil recovery (EOR). The results show that the dynamic imbibition process of tight/shale oil water flooding can be divided into three stages: strong displacement and weak imbibition stage of rapid production of large pores and fractures under displacement action; weak displacement and strong imbibition stage of slow production of small pores and fractures under counter-current imbibition action and dynamic equilibrium stage of weak displacement and weak imbibition. The greater the displacement pressure, the lower the degree of imbibition recovery and the stronger the contribution of displacement, but it is easy to produce water channeling, leading to an early breakthrough, as a result, the recovery increases and then decreases. The higher the permeability and the better the pore throat connectivity, the greater the degree of both imbibition and displacement recovery, and the shorter the percolation equilibrium time and the greater the recovery. Fractures can effectively increase the imbibition contact area between the matrix and water, reduce the resistance of oil and water seepage, and increase the rate of matrix oil release and total recovery. There are differences in dynamic production characteristics and the degree of contribution to recovery at different development stages. Conducting a soaking program after fracturing is beneficial for fully utilizing the effects of fluid imbibition, displacement, and energy storage; also, the key to EOR is to effectively utilize the carrying effect of the backflow fluid and the displacement during the production stage. This study provides theoretical support for the efficient development of tight/shale oil.

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Poster / 21

Acoustic Properties of Hydrate-Bearing Porous Media Based on Electrical-Mechanical-Acoustic Multi-physics-Field Coupling Model

Author: Yunlong Wang[1]

Co-authors: Lanchang Xing [1]; Wei Wei [2]; Weifeng Han [2]

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There are technical difficulties in accurately controlling and evaluating the micro-distribution mode and saturation of hydrate in physical simulation experiments. Limitations exist in the experimental technologies for investigating acoustic properties of hydrate-bearing sediments and establishing interpretation models of reservoir parameters. The acoustic properties of hydrate-bearing sediments are influenced by hydrate saturation and micro-distribution modes, skeleton particle arrangement and shape significantly. Currently, there is a lack of research work on the influence mechanisms of skeleton particle arrangement and particle shape. Three-dimensional numerical models were established for hydrate-bearing porous media based on digital rock physics technology. For the three kinds of hydrate micro-distribution modes (suspension, contact and cementation), finite-element models were established individually based on the method of electrical-mechanical-acoustic multi-physics-field coupling. The effects of micro-distribution mode and hydrate saturation on sound velocity and attenuation of porous media were examined. The results of sound velocity from the numerical and theoretical models were compared. The influences of skeletal particle arrangement modes and shapes on the sound velocity and attenuation characteristics of sediments under different hydrate micro-distribution modes and saturation conditions were explored, and the mechanisms were discussed. It was demonstrated that: (1) when the hydrate saturation is low, the volumetric proportion of quartz sand particles in the diamond-arrangement model is higher than that in the cubic-arrangement model, thus the sound velocity of the diamond-arrangement model is higher; as the hydrate saturation increases, the difference in the volumetric proportion of hydrates between the two models increases and the volumetric proportion of hydrates in the cubic-arrangement model is higher, consequently the sound velocity growth rate in the diamond-arrangement model is lower; (2) the porosity of the diamond-arrangement model is smaller than that of the cubic-arrangement model, and the energy attenuation during the propagation of sound waves is lower; (3) compared with the spherical-particle model, the elliptical-particle model contains more pores with smaller aspect ratios, resulting in a smaller bulk modulus and lower sound velocity; (4) the ellipsoidal-particle model contains more and smaller pores, which results in lower wave-energy loss than that of the spherical particle model. This study may provide a theoretical support for the data interpretation of seismic exploration and sonic logging for natural gas hydrate reservoirs.

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MS08 / **23**

Investigating the limits of averaging: a numerical case study employing diffusion-reaction in porous media

Author: David Rieder[1]

Co-authors: Frank Peters [1]; Hans Kuipers [1]

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Effective descriptions are often utilized to describe mass transfer phenomena in porous media, i.e. in heterogeneous catalysis, filtering or subsurface transport. Besides more than a century of research, the a priori determination of the relevant effective transport parameters has shown to be elusive and is still subject of research. A major challenge is the appropriate mathematical upscaling of the intricate influence of pore-scale phenomena on the Darcy-scale behavior for realistic morphologies. Typically, such upscaling procedures incorporate convenient estimates to determine the significance of the pore scale transport phenomena with respect to the Darcy scale. Often, such estimates are based on the pore space geometry, macroscopic transport properties and external process parameters. A popular example there is the assumption, that the pore side length scale is significantly smaller than the representative dimension of the porous medium.
To gain insight into the applicability of commonly used averaged descriptions with respect to the coarseness of the pore space, direct numerical simulations of diffusion with first order surface reaction in a resolved pore space were employed. There, a 3D resolved model was developed, based on the finite volume approach utilizing a second order implicit immersed boundary method to accommodate the representation of the pore space. The developing transient species profile was monitored and compared with the analytically derived profiles to the complementary averaged problem.
To investigate the limitations of the averaging approach, the numerical model was applied to a variety of model porous media with varying characteristic length scales and particle Thiele moduli. The generated insights concerning the emergence of Darcy scale behavior from pore scale phenomena will be presented and implications discussed.

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Modeling of Dispersive Shear Thinning Polymer-Surfactant Flooding

Author: Prabir Daripa[1]

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In this talk, we will discuss recently developed models of dispersive shear thinning polymer-surfactant flooding. These models are based on Darcy's law, transport equations for the components and non-Newtonian rheology. In the absence of dispersion and shear thinning effects of polymer, this system has been solved numerically by Daripa & Dutta [1]. Recently, shear thinning has been included in the model and this new model has been used to study the effect of shear thinning numerically by Daripa & Mishra [2]. This model is now extended to include the effect of dispersion of polymers. Effect of dispersion through numerical solutions will be discussed in the absence and presence of shear thinning effect. In particular, we study the
effects of shear thinning, anisotropic mechanical dispersion and molecular diffusion on the advective transport of constituents like polymers. Also, we numerically investigate the effect of potentially nonlinear interactions between shear thinning, dispersive transport, capillary effects, and multiscale heterogeneity. Numerical results demonstrating the effects of shear thinning and dispersion on viscous fingering, viscosity waves, and efficiency of polymer-enhanced oil recovery will be presented.

We will also discuss differences between this model and the Hele-Shaw model which has been previously studied by Daripa & Gin [3]. Parts of this talk will be based on joint work with Sourav Dutta and Rohit Mishra.

[1] P. Daripa and S. Dutta, "Modeling and simulation of surfactant–polymer flooding using a new hybrid method", Journal of Computational Physics,vol. 335, pp. 249-282 (2017).

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MS01 / **26**

Visualisation of [11C]CO2 storage in coal with positron emission tomography imaging

Author: YU JING[None]

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CO2 geo-sequestration is a practical approach to achieve net-zero carbon target. Coal has become an optimal geological storage option due to its large adsorptive capability for CO2. However, one of the main challenges for successful CO2 geo-sequestration is the reduced injectivity that are caused by adsorption-induced swelling of coal matrix. In addition, its complex and heterogenous internal pore and fracture structure make the processes of gases adsorbing, desorbing, and transporting more complicated compared with conventional rocks. This work aims to gain insights about the gas transport behaviours in coal by developing a novel experimental framework with Positron Emission Tomography (PET) imaging technology to directly visualise gas flow multiphysics in coal.

PET imaging has demonstrated its capability in providing real-time visualisation of fluids flow in geological materials. However, it has not been used for the study of CO2 injection and storage in coal for the application of CO2 geo-sequestration. To observe the processes directly, [11C] CO2 is the most optimal radiotracer, which is rarely used due to its short half-life (20.4 min) and handling safety issues as a gaseous tracer. In this work, a novel laboratory protocol is developed to use gaseous [11C] CO2 as the radiolabelled tracer to visualise and quantify dynamic processes of gas spreading, adsorption, diffusion, and advection flow in coal under in-situ conditions. The experimental setup integrates core flooding setup with PET scanning. Coal samples are pre-treated to mimic different injection conditions, including coal seam gas reservoirs in early production stage, gas depleted stage and CO2 storage stage. Due to high temporal resolution of PET imaging, time-lapse CO2 gas concentration map of each test is acquired by converting the PET intensity values to gas concentrations. Impacting factors on storage capacity and efficiency are also studied, including permeability, gas adsorption, gas exchange, and initial storage conditions.

This work introduces a new laboratory protocol and analysing framework to quantify sub-core scale multiphysics CO2 flow in coal, which provides a foundation for future across-scale theoretical and experimental study of multiphase and multicomponent flow behaviours in coal for the application of CO2 geo-sequestration.

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MS01 / 28

Effects of Thermal Cycling on Sealing Ability of Sealant Surrounding Steel Pipe for CCS Applications

Author: Kai Li[None]

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In wells designed for carbon capture and storage (CCS), leakage pathways may develop due to thermal cycling when injecting cold CO2 into the warm subsurface, for example, debonding between cement and casing, or fractures in the cement itself. These leakage pathways can impede the permanent geological storage of CO2. In this study, we investigate how thermal cycling affects the sealing ability of cement surrounding steel wellbore casing under unconfined conditions. To this end, cylindrical sealant samples (OD 30 mm, Length 70 mm) with a steel pipe (ID 4 mm, thickness 1 mm, length 110 mm) in the middle, are used to mimic the cement sheath surrounding the casing in the wellbore. We adopt sealants of five different compositions. S1 is ordinary Portland cement (OPC)-based, S2 is OPC-based with ultra-low permeability, S3 is OPC-based with CO2 sequestering additives, S4 is calcium aluminate cement(CAC)-based, and S5 is geopolymer-based.
In the experiments, we mount PVC caps at each end of the sample to isolate the flow channel through the pipe from another flow channel toward the top surface of the sealant. Three thermocouples are installed at the surface of the sealant, inlet, and outlet of steel pipe, separately. The entire sample assembly is placed in an oven. Before thermal cycling, we apply 3 bar N2 on the sealant and monitor its penetration rate through the sealant for 1 hr. Subsequently, we heat the sample at 60 for 1.5 hr. To apply thermal cycling, we inject 5℃ water through the pipe at 80 ml/min for 2 mins, then stop the injection and allow the sample to reheat for 12 mins before the next injection. We repeat this for 12 cycles.
In our study, we haven't observed any cracking in the sealant material itself. This is because the induced thermal stress upon thermal cycling is smaller than the tensile strength of the sealant. Among the five sealants, we found that the bonding performance of S3 on steel is the best. All other sealants were negatively affected by thermal cycling: S1 and S5 experienced more debonding than others, while S2 and S4 experienced minor debonding. The bond strength of all five sealants (including S3) decreases after thermal cycling, further indicating that debonding has occurred. We attribute the magnitude of debonding to be due to a combination of thermal expansion coefficient and Young's modulus. Steel has a high expansion coefficient compared to sealant. Of the tested sealants, S1 and S5 have the lowest thermal expansion coefficients, while S2 and S4 have the largest, i.e. closer to that of the steel. We hypothesize that, during thermal cycling, S2 and S4 expand and shrink with a more similar rate as steel, resulting in a small mismatch in strain and hence less debonding compared to

S1 and S5. Additionally, S1 has the largest Young's modulus, whereas S3 and S4 have the lowest. This indicates that S3 and S4 are more compliant, so S3 and S4 can more easily elastically deform upon thermal cycling, resulting in less damage to the bonding.

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MS13 / **29**

A Multi-Scale Approach for Assessing Shale Oil Accessibility: Digital Core, Molecular Simulation and Machine Learning Analysis

Authors: Yifan Yin[1]; Zhixue Sun[1]

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This study presents a novel multi-scale approach for assessing the accessibility of shale oil in cores. By using FIB-SEM equipment to build digital core, watershed and maximum ball method to extract pore size and shape factor. Then molecular simulation is used to study the availability of shale oil in individual pores with different shapes and radii. Finally, combining the results of the above two scales, machine learning is used to predict shale oil availability across the entire core. On the core scale, the watershed and maximum ball method is used to extract the core pore network model, and it is found that square pores occupy the highest proportion among the three pore types, and most of the radii are distributed in the range of 2-3 nm. The molecular scale dynamic simulation results show that the adsorption forms of shale oil are different in different pores, and the adsorption of shale oil in circular pores is less than that in flat pores. The proportion of shale oil adsorption in square pores is the highest, followed by triangle pores, and the proportion of shale oil adsorption in circular pores is the lowest. The Random Forest machine learning algorithm is used to predict the availability of shale oil with different pore shapes and obtain the shale oil availability ratio of the whole core. The results show that the pores with a more obvious angular structure show a lower shale oil availability ratio. In general, the impact of pore shapes on shale oil availability is not significant, and the difference between different pore shapes is only 10%. The multi-scale evaluation method for shale oil availability proposed in this study is helpful to better understand the availability of shale oil in reservoirs and to optimize recovery strategies.

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MS01 / **32**

CO2-enhanced shale gas recovery –Monotonic and cyclic injection

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The process of CO2 enhanced shale gas recovery CO2-ESGR seeks to recover the maximum amount of shale gas while simultaneously injecting and trapping CO2 to reduce greenhouse gases. CO2-ESGR has been studied in the laboratory and tested in small field prototypes, however, its commercial feasibility remains questionable. Therefore, more fundamental and experimental research need to be conducted (Nuttal et al., 2005; Schepers et al., 2009).
CO2 enhanced shale gas recovery relies on the preferential adsorption of CO2 and uses pressure gradient to displace and produce methane gas (Hughes et al., 2012; Klewiah et al., 2020). CO2 has a higher adsorption affinity compared to methane gas in shale reservoirs (Weniger et al., 2010; Shi et al., 2019). Competitive gas adsorption depends on the gas type, pressure, temperature, water content, mineralogy, organic content and maturity (Liu et al., 2019). Multiple studies have investigated the competitive adsorption of single-or-mixed gases under static conditions (Heller and Zoback, 2014; Zhou et al., 2018; Sun et al., 2020); however, adsorption-desorption under cyclic conditions remains unexplored.
We explore the interaction between CO2 and CH4 with dominant shale components (clay and organic matter) and natural shale specimens under reservoir pressure and temperature conditions (P=10MPa and T=40C). Experiments are designed to identify the interplay between governing parameters for different boundary conditions. The pressure vessel includes separate gas injection systems; an in-line binary gas analyzer measures the produced gas composition. In this presentation, we compare the methane recovery factor for two different injection protocols: (1) continuous flow injection and (2) pressure cycles. Experimental results show a significant increase in methane recovery efficiency driven by CO2 injection, particularly during pressure cycles.
A parallel numerical model takes into consideration gas advection, adsorption/desorption, diffusion and mixing. This numerical analogue allows to comprehend the interaction between ongoing processes, to develop injection/production protocols that optimize methane production and CO2 storage, and to upscale results to the field.

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Conference Proceedings:

MS08 / **33**

Pore-scale digital twin of sorption thermal energy storage in packed bed reactor using a machine-learning assisted dual-network model

Author: Mingliang Qu[1]

Co-authors: Sajjad Foroughi [2]; Jie Luo ; Jinping Yang ; Qingyang Lin [3]; Martin Blunt [3]

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The adsorption thermal energy storage system is widely utilized for low-grade heat storage and recovery due to its environmentally friendly and efficient characteristics. In this work, we utilized a machine-learning assisted dual-network model to construct an upscaling model from micro-kinetics to reactor in order to simulate an adsorption heat release process involving heat and mass transport on a meter-scale packed bed reactor. The simulation results were compared with experimental measurements and analytical models to demonstrate the accuracy of the model in predicting temperature and concentration distribution within the system. Subsequently, we explored the impact of different boundary conditions on the internal state parameters during the adsorption heat storage process, offering valuable insights for the design of adsorption heat storage systems.

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MS09 / 34

Quantification of geometric and flow characteristics for CO2 storage at pore-scale using a DC-GAN based digital experiment approach

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The trapping efficiency of CO2 storage in porous subsurface is influenced by various geometric and flow characteristics. Conducting experimental studies on reservoir structure characteristic parameters and actual storage efficiency consumes a significant amount of resources, making it difficult to analyze the uncertainty of parameters through a large number of experiments. In this work, a deep convolutional generative adversarial network (DC-GAN) was employed to generate 1000 sets of images that are visually indistinguishable by using tomographic images of Bentheimer sandstone as the training data. This is followed by performing image analysis and pore network modelling to obtain geometric (e.g. Minkowski functionals) and flow (absolute and relative permeability, capillary pressure, saturation, and trapping efficiency) properties. With maximum capillary of 7.0 KPa, we found that the trapping efficiency ranged from 32% to 40%. We then explored the uncertainty of all geometric and flow characteristics to determine the minimum number of digital experiments to reproduce the same statics. This work proposes a strategy for coupling deep learning method and pore network models to conduct a large number of digital experiments on complex porous media. This can be used to correct experimental errors obtained through traditional experimental methods and guide the design of geological CO2 storage systems.

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Pore-scale experimental investigation of dry-out effect due to supercritical CO2 injection into saline aquifers

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Carbon dioxide and other heat-trapping "greenhouse" pollutants have continuously and significantly increased in the atmosphere over the past 100 years ago due to the mass consumption of fossil fuels. Carbon Capture and Geological Storage (CCS) is one of the viable solutions for minimizing CO2 emissions into the atmosphere. Nevertheless, there are still challenges and possible consequences associated with implementing this technique. There is substantial concern about the formation dry-out induced by injecting a large amount of dry-supercritical CO2 into the saline aquifer which leads to the vaporization of the resident brine into the CO2 stream and salt precipitation in the near well zone of the reservoir, diminishing the porosity and permeability of this region. Hereupon, this phenomenon is going to affect the well injectivity and pressure build-up adversely.

This research focuses on finding the effects of the dry-out phenomenon on porosity impairment which is usually followed by severe negative consequences like the loss of well injectivity. This study employed microfluidic technology and lab-on-chip experiments to develop a workflow for monitoring and evaluating porosity changes during scCO2 injection into the saline aquifers.

In this study, to determine how porosity changes during a CO2 injection operation, two variables were considered: 1) CO2 injection flow rate and 2) pore network types (shape and size). Thereafter, the selected microfluidic chips (Regular and Irregular) saturated with a specific concentration of the brine solution were exposed to the CO2 injection at different injection flow rates (0.05, 0.1, and 0.2 ml/h). The processed images by Image J software along with data analysis revealed a new insight into the consequences of salt precipitation and subsequent dry-out phenomenon.

Experiments utilizing the PRS chip revealed that as the CO2 injection flow rate increases, more salt is anticipated to precipitate inside the porous media. Contradictory to the experiments employing the PRS chip, salt precipitation in the Regular chip was less evident as the CO2 injection flow rate increased. Investigation of the pore structure effect showed that the salt precipitation inside the PRS micromodel was significantly higher compared to the Regular one because of the grains' shape and angularity. Therefore salt coverage and porosity impairment were more evident for the PRS chip which is probably due to the existence of more evaporation and precipitation sites on the surface of grains.

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MS09 / **36**

Invasion of Porous Layers for Electrochemical Processes: Experimental Studies and Lattice Boltzmann Simulations

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In polymer electrolyte membrane water electrolyzers (PEMWE) and polymer electrolyte membrane fuel cells (PEMFC), efficient electrochemical reactions depend on the optimal flow of water and oxygen within porous electrodes. However, a significant challenge arises due to concentration losses, also known as diffusion overpotential or mass transport overpotential (Vdiff). This phenomenon is attributed to mass transport limitations caused by the counter-current flow of reactants, such as water in PEMFC and oxygen in PEMWE in the pores of the electrodes. This limitation negatively impacts the voltage output, as the electrochemical reactions are not as efficient as they could be. Understanding and addressing these mass transport challenges is essential for improving the overall efficiency of polymer electrolyte membrane-based devices.
Based on the state of the art, Lattice Boltzmann Modeling (LBM) is used to investigate the two-phase flow in the porous transport layer (PTL) of PEMWE and the cathodic catalyst layer (CL) of PEMFC. For the first case, the invasion of O2 in a water-saturated anodic PTL structure (drainage invasion process) is delineated with the implementation of the Shan-Chen LBM for PEMWE. The simulation results are discussed with respect to experimental findings and compared to pore network simulation results. For the second case, the model was tailored for the application to two-phase flow inside an initially empty GDL that is invaded by water at constant current density (imbibition invasion process). For this purpose, evaporation of water was additionally implemented in the LBM imbibition algorithm in order to investigate the relationship between water generation and removal by evaporation. For both studies, reconstructed pore structures from 3D tomography image data was used. We aim to present the overall methodology as well as the major outcomes of this study.

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MS05 / **37**

Microcalorimetric Evaluation of Microbial Activity and Reaction Rate in Sand-packed Porous Media During Microbial-Induced Carbonate Precipitation For CO2 Leakage Remediation

Author: Jacquelin Cobos[1]

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Carbon capture and storage (CCS) is a key technology to reach long-term climate goals that limit the temperature rise to 1.5 ◦C above pre-industrial levels. It consists in capturing CO2 from large industrial
points and geological storage in underground formations, such as depleted oil and gas reservoirs, unminable coal beds, and deep saline aquifers [1]. The success of this technique depends on avoiding
CO2 leakage to the surface through the complex subsurface geometric structures such as faults, fractures, and abandoned wells. Microbial induced calcite precipitation (MICP) is considered as a promising
in-situ method for sealing subsurface leakage paths. This technique utilizes microbes to induce calcium carbonate precipitation, which effectively reduces the porosity and permeability of the porous media,
thereby mitigating CO2 leakage risks [2].

Complex bio-geochemical interactions considering rock-microbes-reactant solution are needed to get a broad assessment of MICP efficiency in geological porous media. However, this is not an easy task
due to the complexity of the microbial activity and rock-forming minerals. In this study, we aim to understand the impact of particle size, specific surface area and pore volume on microbial activity and
geochemical rates during MICP. An extremely sensitive microcalorimetry technique called Isothermal titration calorimetry (ITC) is used to assess the microbial activities and reaction rates within various
water-saturated reservoir rocks inoculated with bacterial solutions [3]. In the ITC experiments, 100 mg of sandstone particles with different size was placed in a reaction vessel and 200µL of bacterial solution (sporosarcina pasteurii stains) was added to the rock particles [4]. The titration ampule containing the rock-bacterial solution was lowered stepwise into the calorimeter and equilibrated for 1 hour at 35 ◦C.
Seven injections of 9.948 µL of the reactant solution (calcium chloride solution) were titrated with a time interval of 420 seconds into the slurry to determine the bio-geochemical reactions by monitoring heat
changes. A quasi-2D sandpack (Fluidflower) was used to identify CO2 flow patterns after MICP treatment [5].

This work shows that the bio-geochemical interactions are exothermic (thermodynamically favorable) and therefore proceed spontaneously. The reaction activity within sandstone is 10 to 18 times

higher than in corresponding bulk solutions. This observation underscores the significance of available surface area in influencing both microbial colonization and the speed at which reactions occur in the MICP process.

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MS04 / 39

Unified surface poromechanics theory capturing condensation-induced contraction of mesoporous materials

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The phenomenon of adsorption-induced deformation is prevalent in both natural materials such as wood and coal, as well as in engineered materials like cement, MOFs (Metal-Organic Frameworks), and porous polymers. As the partial pressure of adsorbate vapor rises, the strain isotherm of these materials can display intricate nonlinear and non-monotonic behaviors.

Under low partial pressures, most porous materials undergo volumetric expansion. This expansion can be attributed to the reduction of surface stress and the subsequent relaxation of adsorption stress experienced by the solid skeleton—a phenomenon commonly known as the "Bangham effect." This effect is well-described by the surface poromechanics formulation proposed by Zhang (2018). For microporous materials, early adsorption can lead to a subtle shrinkage before the onset of swelling. This is linked to the development of negative disjoining pressures in nanopores, as explained by Eskandari-Ghadi and Zhang (2021).

Despite these advances, the current surface poromechanics formulation is only for a single-phase pore fluid and therefore, does not apply to partially saturated porous media nor capture the dynamics of phase transition of the pore fluids. For this reason, it is unable to model the sudden contraction of mesoporous media at intermediate vapor pressure levels induced by capillary condensation. This contribution outlines our progress toward developing a unified surface poromechanics formulation that meets the following criteria:
1. It takes into account the phase transition of pore fluid from vapor to liquid and the emergence of the liquid-vapor interface.
2. It accurately reproduces the water retention characteristic curve unique to each porous system.
3. It captures both the early Bangham expansion (without condensation) and the significant contraction resulting from condensation in a consistent manner.
4. The theory's asymptotes at degrees of saturation equal to 0 and 1 align with the conventional poromechanics theory for single-phase pore fluid.

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MS09 / **41**

Pore scale characterization of dissolution process during CO2 injection in sandstones: an simulation study

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Dissolution trapping is one of the crucial trapping mechanisms for geological carbon storage in deep saline aquifers. The injected supercritical CO2 (scCO2) flow and dissolution processes are coupled and interact with each other. Therefore, we performed direct numerical simulations in three-dimensional micro-CT images of sandstones using the volume of fluid and continuous species transfer method. We investigated the coupled scCO2 flow and dissolution processes at pore-scale under different rock structures, capillary numbers, and rock wettability conditions. The dynamic evolution of the scCO2/brine phase distribution and scCO2 concentration distribution occurring during the injection period were presented and analyzed. Complicated coupling mechanisms between scCO2-brine two-phase flow and interphase mass transfer were also revealed. Our results showed that the scCO2 dissolution was highly dependent on the local distribution of scCO2 clusters. The rock with relatively high porosity and permeability would have more capacity for scCO2 injection resulting in a faster and greater dissolution of scCO2 in brine. The effect of capillary number on the scCO2 dissolution process was related to the range of capillary number. Rock wettability was found to be another factor controlling the scCO2 dissolution process by affecting the scCO2-brine interfacial area. Our pore-scale study provides a deep understanding of the scCO2 dissolution trapping mechanism, which is important to enhance the prediction of sequestration risk and improve sequestration efficiency.

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MS01 / **42**

Realistic evaluation of prototypical porous materials for carbon capture

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Carbon capture, utilization, and storage (CCUS) is an attractive approach to help decarbonization from point sources, like energy supply and other industries, as well as for pulling CO2 out of the atmosphere (i.e., direct air capture, DAC). Among several approaches at differing technology readiness levels, solid sorbents are promising as they generally combine high uptakes and selectivity with milder regeneration energies.

Adsorption screening and testing of promising materials are often performed using pure component or point uptake experiments, which only give information about adsorption capacity and ideal selectivity. At realistic process conditions, competitors such as moisture and temperature have a large effect on the uptake of CO2, wherein the presence of water could either increase CO2 capacity, compete for the same adsorption sites, or even induce material collapse. The kinetics on the other hand is another important factor for an effective separation.

Figure 1 shows that apparent CO2 uptake decreases by 5% RH in Zeolite 13X. Figure 2 presents the details of the sorption kinetics of both components highlighting replacement effects.

In this work, several porous materials including zeolites, MOFs, and functionalized resins are screened in realistic conditions for CO2 capture using advanced dynamic gravimetric sorption and breakthrough methods. The tests were conducted under varied conditions, e.g., different CO2 concentrations and relative humidity. The results showed that humidity is the key factor affecting the CO2 capture efficiency. This study provides a reference for screening the effective sorbents for carbon capture.

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Poster / **43**

Nanomechanical properties of Janus nanoparticle-stabilized Pickering emulsion in confined nanochannels

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Co-authors: bo wang [2]; fanhua zeng [1]

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The crucial role of the interaction between Pickering emulsions and confined nanochannels in their industrial applications is well acknowledged. However, there is a limited understanding of how the modulation of deformation stability and rupture limits of Pickering emulsions occurs when they come into contact with solid walls, particularly in relation to the influence of solid particle shells. This study employs molecular dynamics (MD) simulations to elucidate the nanomechanical properties of Pickering emulsions stabilized by Janus nanoparticles (JNP) in confined channels. For the first time, a comprehensive predictive model is developed to characterize the contact behavior of Pickering emulsions with surfaces exhibiting distinct wettability. The contact stress experienced by an emulsion is found to be dependent on factors such as the equivalent elastic modulus of the emulsion, geometric deformation function, and the influence of the JNP shell along with its interactions. Additionally, it is observed that hydrophobic surfaces induce the rupture of Pickering emulsions under compression. The delay in rupture is achieved by increasing the surface coverage (ϕ) of JNP. Notably, when ϕ reaches a critical value, the JNP shell can assume an ordered quasi-solid structure, leading to a significant enhancement in emulsion stability. These findings have practical implications for the design and screening of specific Pickering emulsions, especially in applications such as enhanced oil recovery, drug or food delivery, and cosmetic ingredient absorption, where the management of deformation and rupture on solid surfaces is crucial.

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Poster / 44

Investigation of pore-scale evaporative drying, salt precipitation and crystallization migration in CO2 injection process by a lab-on-a-chip system

Author: BO WANG[1]

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The current research work mainly focuses on the NaCl-based formation brine, and the influence of different types by formation brine on the salt precipitation have not yet been investigated. Also, the damage effect of local salt crystals on the pore structure and the migration mechanism of salt crystals after precipitation remains unclear. Based on this, this study aims to investigate the effect of different brine types on salt precipitation and migration in CO2 injection process.
In this study, a pore-scale CO2 displacement experimental study was performed using a visualized microfluidic model. Dry CO2 was injected into homogeneous and heterogeneous microchips saturated with different simulated formation brine solutions (NaCl/CaCl2/NaCl-CaCl2) at a set flow rate. Then, the two-phase flow, water evaporation, salt growth, crystallization and migration processes in the pore scale were observed under brightfield imaging using advanced polarizing microscope and X-ray microtomography imaging technology. Finally, fluorescence and transmission imaging techniques were used to clarify the distribution of salt precipitation and to quantify the amount of salt crystal.
The results indicated that the brine after CO2 flooding formed four types of irreducible water, which are liquid bridges, domes, connected liquid pools and independent liquid pools. With the increase of CO2 displacement volume, cubic regular crystals and irregular microcrystals formed inside the chip saturated with NaCl solution, which is consistent with the existing literature research. However, in our study, we also observed a new form of salt precipitation—salt bridge aggregates. Compared with the above two salt precipitation forms, salt bridge aggregates are more likely to block the pore structure, thereby affecting the permeability of the near-wellbore area. In contrast to the chip of saturated with NaCl solution, the chip saturated with CaCl2 solution did not observe an obvious solid-phase crystal structure. However, we observed an unprecedented phenomenon—the thickness of the water film was significantly reduced, and finally viscoelastic water film salt and aggregates were formed. In addition, the results of fluorescence quantification of salt crystals also observed the self-enhancement effect of salt crystal growth and the water film salt transport effect, which synergistically strengthened the precipitation rate and amount. This study comparatively analyzes the influence of brine type on salt precipitation, which provides new insights for in-depth understanding of the effect of salt precipitation on CO2 injection capacity.
We provide new insights into the dynamics of pore-scale salt precipitation through visualized microfluidic experiments and identify possible explanations for the large-scale salt precipitation observed in situ. In addition, the salt precipitation mechanism and migration characteristics of different brine types may provide new suggestions for future numerical simulation research, and provide criteria for accurately predicting the distribution of salt precipitation and its impact on reservoir physical properties.

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MS09 / **45**

Micro-Continuum Modeling of Mineral Nucleation and Precipitation at Pore-Scale

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Mineral nucleation and precipitation commonly occur in nature and plays an important role in many energy-related applications with reactive flow, especially, at pore-scale. For instance, minerals nucleate and precipitate as scale in the pore structure in unconventional reservoirs and significantly reduce the permeability of the porous media. This phenomenon could lead to a rapid decrease in production and cause significant financial loss. The need to predict the dynamic properties of such systems has resulted in questions about the fundamental mechanisms of reactive flow as well as mineral nucleation and precipitation in pores. Additionally, there is still a discrepancy between laboratory molecular scale findings and large-scale observations. To address this discrepancy, modeling methods at the pore scale started gaining interest recently due to the capability of capturing reactive and nonreactive species transport, effects of pore topology, and interface chemical reaction within the same approach, which typically is difficult to observe directly in experiments.
For some solutions, especially high saturation index solution, the nucleation process could potentially play an important role in the precipitation due to either heterogeneous or homogenous nucleation, which was largely overlooked in most previous numerical models for mineral precipitation. In this study, we coupled the micro-continuum simulation approach based on Darcy-Brinkman-Stokes (DBS) equation with the classic nucleation theory (CNT) to study the stochastic nucleation process in reactive flow. A range of different parameters were studied to understand their impact on the nucleation process and precipitation. It was discovered that such a nucleation process was affected by the Damköhler number and Peclet number as well as other effects. As the precipitation reaction on the crystal surface enhances, the total amount of nucleus formed on the substrate decreases due to the depletion of species in the vicinity of the substrate. In general, the competition between flow/transport of species and precipitation consumption governs the behavior of phase change procss and produces different scenarios. The results of this study are expected to shed light on the mechanism of liquid-solid interaction within porous medium.

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MS09 / **46**

Numerical simulation of two-phase flows in digital core samples with underresolved porosity

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Micro-CT scans are widely used for rock models in Digital Rock Physics applications. However, up to one-half of the connected porosity of carbonates and shales is underresolved with micro-CT due to the small pore size. This underresolved pore space may still support multiphase fluid flow. To

simulate two-phase flows in models where both large-scale and underresolved pores are present, we developed a numerical algorithm based on the combination of the phase-field model with two-phase filtration, which supports continuous phase transport in a multi-scale pore space.
The fluid flow is simulated using the unified Navier-Stokes-Brinkman equation, which is well suited for the models where the absolute permeability is at the level of mcroDarcy, which is the case for the underresolved porosity of carbonates and shales. This equation is solved using the projection-based method. The phase transport in the resolved pores is governed by the Cahn-Hilliard equation of the phase field, which makes it simple to treat the complex geometry and topology of the pore space and the phase. Phase transport in the underresolved pores satisfies the two-phase filtration equation, accounting for the capillary pressure. The two models are coupled at the interface between the resolved and underresolved pores based on flux continuity. Additionally, the wetting-angle boundary condition is satisfied for the phase-field model.
The designed algorithm and its GPU-based implementation are used to estimate the relative permeability and capillary pressure of the samples with underresolved porosity.
The research was supported by RSCF grant no. 21-71-20003

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MS12 / 47

Prediction of CO2 Injectivity into Low-temperature Water Zones below Natural Gas Hydrate Reservoirs for Non-Leaking Storage

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Abstract

The potential leakage of carbon dioxide (CO2) from traditional underground carbon storage reservoirs has become a growing concern. This study suggests a novel approach —injecting CO2 into subsea water zones situated under natural gas hydrate reservoirs. The objective is to store CO2 within the water zones in hydrate form, thereby minimizing the risk of future CO2 leaks. Assuming a sufficiently rapid flow of CO2 during injection to prevent hydrate formation, an analytical model was developed to predict well's CO2 injectivity. The case study utilizing data from the natural gas hydrate reservoir in the Shenhu area, Northern South China Sea, indicates that the CO2 injectivity of a water zone underlying a natural gas hydrate reservoir is significantly influenced by the transmissibility of the water zone. With water zone transmissibility values varying within a range of -50% to +50% around the mean value of 15.79 Darcy-cm, well injectivity is projected to be nearly proportional to water zone transmissibility, ranging from 6 tons/day to 16 tons/day. Interestingly, CO2 injectivity in the water zone exhibits minimal sensitivity to the permeability of the natural gas hydrate reservoir. In the examined case, the anticipated CO2 injection rate is expected to vary only slightly, ranging from 10.5 tons/day to 11.5 tons/day, even with a permeability uncertainty of

the gas hydrate reservoir ranging from 1 md to 3 md. The injectivity of a well completed in the water zone aligns with that of a well completed with frac-packing in the natural gas hydrate reservoir. Both types of wells are anticipated to inject CO2 at a flow rate ranging from 6 tons/day to 16~17 tons/day, contingent upon the transmissibility of the water zone and the transmissibility of the hydraulic fracture. Notably, injecting CO2 into water zones, as opposed to frac-packed natural gas hydrate reservoirs, offers the advantage of cost savings by eliminating the need for hydraulic fracturing.

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MS05 / **49**

Bioclogging during underground hydrogen storage: Assessing impact of biofilm formation on hydrogen injection and recovery.

Author: Na LIU[1]

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In response to the urgent global concerns regarding climate change, there is a critical need for the evaluation and implementation of reliable renewable energy solutions. To bridge the energy demand-supply gap, immediate research into effective energy storage methods is imperative. The use of green hydrogen, generated via renewable electricity's electrolysis, is receiving increased attention, owing to its low volumetric calorific value (3 kWh/m3) and high mass energy density (33.3 kWh/kg). Hydrogen gas as an energy carrier can be stored in large amounts in subsurface reservoirs, such as salt caverns, saline aquifers, and depleted hydrocarbon reservoirs. However, even at minimal aqueous concentrations, hydrogen serves as an attractive electron donor for subsurface microorganisms, including methanogens, sulphate-reducers, homoacetogenic bacteria and iron (III)-reducers. Microbial growth in porous media leads to biofilm formation, narrowing the rock pores and causing potential bioclogging. Therefore, assessing these microbial effects in underground hydrogen storage is crucial to estimate risks associated with gas injectivity, loss, and recovery in large-scale operations.
This study investigated hydrogen consumption by two sulphate-reducing microorganisms in a pressurized microfluidic chip at 10-100 bar and 37 ℃, mimicking conditions akin to shallow gas reservoirs. The microbial cells congregated at the interface of the aqueous phase and hydrogen gas, utilizing the hydrogen to form biofilms. However, bioclogging resulting from biofilm formation was observed when utilizing Lactate as the carbon source, while no such clogging was observed with hydrogen gas. Under the microscope, the comparison between biofilm formations using Lactate and hydrogen gas revealed notable differences. The Lactate-formed biofilm appeared denser and tightly packed, whereas the hydrogen gas-formed biofilm displayed a crystal-like structure. Further analysis with Raman spectroscopy uncovered disparities in the protein structures within these biofilms.After one week of cultivation in a hydrogen-rich environment, the biofilm appeared to detach from the pore

network following the second hydrogen injection drainage. Our hypothesis proposes that this reduction in the biofilm might be due to a shift in bacterial behavior, potentially transitioning from a biofilm-mode to a planktonic-mode state in an environment abundant in hydrogen. Biofilm formation and its adhesion to solid surfaces directly impact wettability, notably increasing hydrophobicity. This change in contact angles leads to a decrease in capillary entry pressure during hydrogen injection, thereby improving drainage efficiency.
These findings emphasize the substantial impact of biofilm dynamics and wettability changes on the efficiency of hydrogen injection and recovery processes in subsurface reservoirs. The results offer critical experimental evidence concerning the microbial risks linked to underground hydrogen storage, thereby contributing to the validation of the upscaled model within this context.

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MS01 / 50

Optimization of porous structures via machine learning for solar thermochemical fuel production

Authors: Da Xu[1]; Meng Lin[1]

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Optimization of the porous structure is essential to achieve high solar-to-fuel efficiency in solar thermochemical fuel production. The porous structure directly converts concentrated solar radiation into heat and facilitates heat and mass transfer, as well as provides sites for chemical reactions. An ideal porous structure is expected to have a large surface area to provide reactive sites, a large mass loading to provide reactants, a small pressure drop in fluid space to facilitate gaseous mass transfer, and uniform solar energy absorption to guarantee thermo-mechanical stability. These optimization objectives demand a comprehensive understanding of the transport and conversion processes in porous structures. The direct 3D multiphysics model based on real morphology is time-consuming and costly to solve. Its further coupling to a conventional optimization algorithm, such as the gradient descent method for structure optimization, is challenging. The triply periodic minimum surface (TPMS) structures are known for their well-defined mathematically controllable morphology and designing flexibility, providing great easiness in structure optimization, so they are introduced into the optimization. In this study, we introduced a machine learning-aided porous structure optimization method for solar thermochemical fuel production. The machine learning tool was used to link the TPMS structures' design parameters with the fuel production performance, temperature gradient, and gaseous flow pressure drop. The training data were calculated from a direct pore-level multiphysics model with various uniform and gradient 3D TPMS structures. The reaction model in this study considered both charge carriers' bulk diffusion and surface reactions, enabling the investigation of the material's kinetics on fuel production performance. The model framework can hence be utilized for porous structure optimization as well as guiding material choices for high-performing solar thermochemical fuel generation.

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Ensemble Variational Bayesian Uncertainty Quantification for High Dimensional Nonlinear Parameter Inversion of Darcy Flows in Porous Media

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The inversion and uncertainty quantification of parameters associated with governing PDEs are important in many scientific and engineering problems. For example, petroleum reservoirs are typically heterogeneous and uncertain due to the sparsity of hard data, and the uncertainty quantification of physical parameters associated with the governing PDEs of flows in porous media, given production history data, is a necessary step before reasonable forecasts can be made. Conventional history matching inversion methods are generally point-estimate, while uncertainty quantification using MCMC is computationally expensive. In the current study, an efficient ensemble variational Bayesian (EVB) uncertainty quantification method is developed for inverting high-dimensional parameters for the governing PDEs. Variational Bayes inference approximates the posterior using trial distributions such that the Kullback-Leibler divergence between the true posterior and the trial distribution can be minimised. In EVB, a reduced-order model is built using principle component analysis to enhance the convergence of small-size ensembles. The trial distribution is optimized simultaneously as the ensemble of realizations are updated by data assimilation. In particular, particle filtering is adopted for the nonlinear inverse problem under consideration. Two- and three-dimensional test cases of single- and two-phase Darcy flows in petroleum reservoirs are presented for validation.

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pulsating seepage and thermal deformation by injecting high-temperature steam into coal for thermal CBM recovery

Author: zhiqiang Li[1]

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Chinese coal reservoirs are characterized by low pressure and low permeability, which call for enhancement to increase production. However, conventional methods of permeability enhancement can only increase the permeability in fractures, but not the ultra-low permeability in coal matrices. Attempts to enhance such impermeable structures lead to rapid attenuation of gas production, especially in the late stage of gas extraction. Thermal stimulation by injecting high-temperature steam is a promising method that is expected to increase gas production. The critical scientific challenges that still hinder its widespread are related to the evolution law of permeability of high-temperature steam in coal and the thermal deformation of coal. As part of this study, we developed an experimental approach to explore the high-temperature steam seepage coupled with the thermal deformation in coal under triaxial stress. The tests were conducted using cylindrical coal specimens of $\phi 50 \times 100$ mm. The permeability and thermal strain in coal were investigated when high-temperature steam was injected at 151.11 ℃, 183.20 ℃, 213.65 ℃ and 239.76 ℃, respectively. The experimental results revealed, for the first time, that as the amount of injected fluid increases, the steam permeability presents periodic pulsation changes. This paper introduces and explains the main traits of this discovery that may shed more light on the seepage phenomenon. When the injected steam temperature increases, the amplitude of pulsating permeability decreases, the frequency increases, the period becomes shorter, the pulsation peak appears earlier, and the stabilization time becomes longer. The average peak permeability shows a "U-shaped" trend that decreases and then increases as the steam temperature increases. Meanwhile, with the extension of steam injection time, the axial, radial, and volumetric strains of coal show a stage-wise expansion characteristic at different temperatures of steam injection, except for the radial strains at 151.11℃. A two-phase flow theory of gas-liquid is adopted to elucidate the mechanism of pulsating seepage of steam. Moreover, the influencing mechanism of inward and outward thermal expansion on the permeability of coal is interpreted. The results presented in this paper provide new insight into the feasibility of thermal gas recovery by steam injection.

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MS15 / **57**

Application of Machine Learning and Deep Learning Methods in Reservoir Development

Authors: Kai Zhang[1]; Jinding Zhang[2]; Qinyang Dai[2]; Xinyan Wang[2]; Guojing Xin[2]; Liming Zhang[2]; Xia Yan[2]; Piyang Liu[3]; Huaqing Zhang[2]; Yang Wang[3]; Wenjuan Zhang[3]

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Machine learning (ML) has revolutionized various aspects of underground seepage, geological modeling, reservoir numerical simulation, production optimization, and big data analysis in the oil and gas industry. In particular, when it comes to reservoir development, ML methods, e.g., deep learning (DL) and intelligent computing, have proven to be superior to traditional methods in terms of effectiveness and efficiency. Our study focuses on the application of cutting-edge ML methods to real-time reservoir optimization problems. The research includes reservoir history matching, well placement optimization, production optimization, wellbore fault diagnosis, big data analysis, and so on. Through extensive research and experimentation, we have observed that ML-based methods, especially DL methods, not only enhance the performance of traditional techniques but also significantly reduce the computational effort. They can quickly give reliable prediction results for variables of interest almost within seconds. ML-based methods can also accurately predict the performance of stimulation measures in oilfields, where an ML-based model is obtained with only available data, instead of expert knowledge in oilfields utilized in traditional patterns. These findings demonstrate the immense potential of ML methods in improving the performance of traditional techniques, providing valuable insights for practical oilfield management and development.

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MS19 / **58**

Electrical response during drying and imbibition of mesoporous materials.

Author: Mariia Liseanskaia[None]

Co-authors: Patrick Funnemann [1]; Michael Froeba [1]; Andriy Yaroshchuk [2]; Patrick Huber [3]; Manuel Brinker [4]

[1] *University of Hamburg*

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Upon the contact of the conductive mesoporous material with an aqueous electrolyte solution, ions adsorb on its surface, spontaneously forming an electrical double layer. In this case, due to the absence of an applied external potential difference, while the total charge of the system is zero, there

is already accumulated a local charge at the interface. The number of adsorbed ions is determined by the chemical composition of the material, the bonds on the surface and, due to the spontaneity of this process, to a large extent by the surface area. Therefore, mesoporous materials with high specific surface area and porosity become the most favorable objects for research. However, when a second electrode with a different surface chemistry is introduced into the circuit, a potential difference occurs. This leads to spontaneous charge redistribution between the electrodes and rearrangement of ions at the interface. Current relaxation and potential difference evolution are the key characteristics of this process. Changes in the imbibition parameters as well as decreasing of wetted surface area during drying affect these electrical responses. Here we investigate the nature of these electrochemical processes and their correlation with fluid dynamics using gravimetric mass uptake measurements in combination with Zero Resistance Amperometry and other Open circuit methods.

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Application of Diffusion Models to Generate Multiphase Fluid Pore-Scale Images

Author: Linqi Zhu[1]

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Generative Adversarial Networks (GANs) have been a typical example of how machine learning has been successfully applied, using three-dimensional images as training datasets, to generate realizations of the pore space, as well as to produce super-resolution images. We further this work with a new generative model: diffusion models (DMs), to generate images of both the pore space and two fluid phases within the pore space, using experimental high-resolution three-dimensional X-ray images of the pore space and fluids at different fractional flows as training datasets. We demonstrate that using DMs, we can generate images for a range of saturations and compare the quality of these realizations against experimental data in terms of Minkowski functionals: saturation, interfacial area, mean curvature, and connectivity (Euler characteristic), as well as contact angle. DMs are a very promising algorithm type for the study of multiphase flow in porous media, with effectiveness comparable to, if not surpassing, GANs. We discuss the use of this methodology to complement pore-scale displacement and imaging experiments, to generate images of arbitrary size and for a wide saturation range. These images provide a basis for further analysis and pore-scale modeling, including the prediction of averaged multiphase flow properties, such as capillary pressure and relative permeability.

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MS03 / 60

A tensorial representation of the hydraulic aperture of rough fractures under compressive and shearing stresses

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The interplay between fracture roughness, topology, and permeability is of major interest in hydrogeology, and models that account for the roughness and tortuosity of fractures to upscale hydraulic apertures that represent the microscale aperture distribution have been the focus of many studies in the past decades (He et al., 2021). However, these models often overlook the tensorial aspects of hydraulic aperture, focusing instead on scalar aperture models (Smith & Freeze, 1979; Neuzil & Tracy, 1981; Schrauf & Evans, 1986; Nick & Bisdom, 2018), which do not fully capture the anisotropy that may be observed in the fluid flow in fractures (Nick & Bisdom, 2018). To address this gap, our study introduces a method for upscaling microscale aperture distributions into equivalent hydraulic aperture tensors.

Constraints in experimental designs limit hydraulic aperture measurements in fractured media to a single direction (Xing et al., 2021; Phillips et al., 2021), preventing the direct verification of hydraulic aperture tensors in the lab. To overcome this challenge, we test our method through numerical experiments. Our approach involves creating synthetic fracture walls using fractional Brownian motion (Mandelbrot & Van Ness, 1968) with varying joint roughness coefficients (Barton et al., 1985). We then use fluid flow simulations to explore the effects impacts of compressive and shear stresses, translated into contact area and shear displacement, on the hydraulic aperture tensors.

Our findings indicate that highly anisotropic fluid flow patterns might emerge due to changes in the contact area between fracture walls, which scalar aperture models cannot capture. In addition, no clear correlation between the JRC values and the anisotropy change with contact area was observed, meaning that more information is necessary for characterizing the flow properties of rough fractures. The flow model used in this research has been previously verified through laboratory tests (Konzuk & Kueper, 2004) and numerical experiments (Rybak & Metzger, 2020), and the upscaling methodology has been validated using analytical solutions (Ferreira et al., 2022). This supports the reliability of the present study, thus suggesting the necessity of a tensorial representation for hydraulic apertures. This work provides a basis for developing a rigorous upscaling methodology utilizing a tensorial representation for the hydraulic aperture.

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Conference Proceedings:

Poster / 63

Pore-scale and Reservoir-scale Investigations on H2 Trapping: Impact of Temperature and Salinity

Authors: Haiyang Zhang[1]; Yihuai Zhang[2]; Mohammed Saad Al Kobaisi[3]; Md Motiur Rahman[3]; Muhammad Arif[1]

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Underground H2 storage is arguably considered one of the promising techniques to achieve net-zero emissions goals. The storage of H2 in geological formations is influenced by a complex function of the physicochemical, petrophysical, and geo-mechanical characteristics of the H2/brine/rock system. This results in the existence of different trapping mechanisms (e.g., residual and dissolution trapping), which will lead to the loss of H2 within the formation. Therefore, it is important to understand the trapping of H2 at different scales to provide a better understanding of the H2 withdrawal efficiency.

To this end, contact angles and interfacial tensions of the H2/brine/sandstone at different temperatures and salinities were collected for the pore network modeling to investigate the pore-scale H2 trapping behaviors. The obtained results were then fitted using the Land trapping model. Subsequently, these trapping behaviors and different H2/brine properties, including density, viscosity, and H2 solubility under different conditions, were then considered in the field-scale simulations. One single injection and production well and four annual injection-withdrawal cycles were considered. The results indicate that a higher temperature leads to less residual trapping in both pore-scale and reservoir scale. The higher temperature and higher salinity conditions are more favorable for H2

production (i.e., a higher H2 recovery factor). In addition, the H2 dissolution trapping is also influenced by the temperature and salinity, which contribute to a maximum of ~5% H2 loss. Furthermore, the H2 plume migrations are also influenced by different temperature/salinity conditions.

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MS15 / 64

Predicting ultimate hydrogen production and residual volume during cyclic underground hydrogen storage in porous media using machine learning

Author: Raymond Mushabe[1]

Co-authors: Sandve Tor [2]; Kane Birane [2]; Donald Wendpanga [3]; David Marban [2]

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In the context of climate change mitigation, underground/subsurface hydrogen storage (UHS) is regarded as a solution that could help tackle the imbalance in renewable energy supply. Excess energy can be stored as molecular hydrogen (H2) and re-used when it is needed. To enable large-scale storage in underground geologic formations, reservoir simulation of cyclic loading scenarios will be used to optimize the storage operations. Hydrogen storage in geological reservoirs involves many physical phenomena related to reservoir dynamics, trapping mechanisms, and potential reactions with minerals and bacteria. Simulating different scenarios of fast H2 injection and production while considering those physical constraints and optimized economic and operational parameters generates loads of data and therefore requires high computational power. The nature of UHS operations and the underlying storage reservoir physics make variations in the generated data sets extensive. Predictive tools like machine learning (ML) that are data dependent can to some extent fill the knowledge gap while simultaneously making the operations more viable. It is therefore interesting to develop tools that can predict parameters associated with fast cyclic operations while minimizing the computational cost. Such methods could help optimize storage operations and reduce operational costs. The work summarized in this abstract attempt to showcase how machine-learned models trained with data generated from simulated UHS systems in porous media can be used to predict ultimate hydrogen production. The same approach is applied to predict H2 amounts that remain trapped in the reservoir due to physics-related parameters. The OPM flow reservoir simulator is used to build models encompassing physical and dynamic parameters to generate cyclic field data which are then used to train time series neural network (NN) models. In the presented work, the reliability and accuracy of the model are ensured through hyper-parameter tuning and cross-validation analysis on a windowed time-series NN. The results obtained in the study show the relevance of machine learning (ML) methods in predicting ultimate H2 production and residual H2 amount in geological

reservoirs. The trained models captured the data trends with mean squared error (MSE) and mean absolute error (MAE), commonly termed as loss functions, from training and validation steps used as accuracy metrics. In one of the reservoir-scale cases, the machine-learned training and predictions in a physics-oriented approach reduced the computational time by about 6773% in comparison with simulation runs by OPM flow on a 4-layer reservoir model. The accuracy metrics and predictions are even much better on simulation data obtained with a one-layer model having a horizontal well along its top and based on a complex cyclic schedule. By showing how machine-learned models can capture some of the complex physical uncertainties associated with underground/subsurface hydrogen storage, our research aims to bring a technical contribution to the development of this technology. Field-scale simulated production and injection data are used to train the models. The paper therefore presents the methodology followed, results from the machine learning methods, and the outlook for future tasks.

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Sarah Eileen Gasda

MS13 / 65

Molecular dynamics investigation of water-gas two phase flow in rough clay nanopores

Authors: Ying Bi[1]; Youzhi Hao[1]; Xiaotian Jia[None]; Detang Lu[None]

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The gas-liquid two-phase flow in rough nanopores plays a crucial role in shale gas extraction. To deeply understand the flow mechanisms, molecular dynamics simulation (MDS) method is often employed to simulate fluid flow in nanoscale channels. However, current researches on two-phase flow at the nanoscale have mainly focused on smooth channels. In addition, accurate simulation of the rock wall material is challenging. This work aims to investigate the mechanisms of gas-liquid two-phase flow in rough shale nanopores by using MDS.
A new rough surface model is constructed by illite crystals, and the water-gas two-phase flow is simulated in it which can achieve a more accurate characterization of flow phenomena in microscale shale reservoirs. To better represent the actual formation conditions, rough nanopores are constructed by adding roughness elements to smooth wall surfaces. Methane and water molecules are introduced into the pore models. The flow process is simulated using the EF-NEMD method. Based on these, the effects of rough particles, different arrangements of rough particles, and varying relative roughness on two-phase flow are investigated. The simulation results reveal that rough particles have a significant impact on gas-water two-phase flow. Statistical analysis is used to quantify the density, velocity distributions and boundary conditions in two-phase flow.
Simulations performed under different roughness conditions demonstrate: the presence of rough particles leads to three adsorption layers of water molecules near the pore walls; it also induces a phenomenon similar to macroscopic Jamin effect during two-phase flow, which severely affecting the flow velocity. Another important observation is that compared to smooth channels, the

presence of rough particles significantly increases the boundary slip length i.e. the thickness of the immobile water layer. The different arrangements of rough particles will generate different negative slip lengths. Furthermore, with the roughness decrease the influence of rough channels on gas phase flow is negligible in hydrophilic channels. The aforementioned findings provide valuable insights into the gas-liquid two-phase flow behavior in rough nanopores, which is crucial for understanding and optimizing the transport and mass transfer processes in nanoscale systems.
This work simulates water-gas two-phase flow in rough nanopores constructed by illite crystals, which has not been previously explored. The major contribution of this work lies in analysing the impact of roughness elements on two-phase flow through MDS. It provides a basis for the development of subsequent mathematical models. Simulating the actual shale reservoir can guide the optimization of production measures. These findings provide insights into the intricate dynamics of gas-liquid two-phase flow in rough channels and contribute to a better understanding of fluid transport in porous media with real-world applications, such as shale reservoirs.

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MS17 / 66

Lattice Boltzmann simulation of water distribution and its effect on methane adsorption in nanoporous shale

Authors: Tao Zhang[1]; Yulong Zhao[1]

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Water vapor sorption in nanoporous media with complex pore structures, such as shale, remains poorly understood. Moreover, the initial water saturation in shale gas reservoirs affects methane's adsorption capacity, posing a challenge for accurate gas reserve estimation. Current methods, including molecular dynamic simulation, sorption experiments, and analytical modeling, have limitations in intuitiveness, research scale, and idealism, respectively.
To tackle this issue, a pseudopotential lattice Boltzmann method (LBM) is developed to explore water sorption and its impact on methane adsorption. This LBM model integrates long-range molecular forces using a modified Shan-Chen model based on the Carnahan-Starling equation of state. Validation of the LBM's simulation for water vapor sorption includes assessments of liquid/vapor densities in phase separation, vapor pressure around liquid droplets, and film thickness in parallel nanoslits using disjoining-pressure theory. For methane sorption, the LBM's validation involves lattice density functional theory and methane sorption experiments.
The findings reveal that water films in nanopores create a liquid pressure disparity of up to 100 MPa between confined and free states. Traditional adsorption theories based on simplistic pore shapes do not apply to nanoporous systems with complex geometries. In inorganic matter, hydrophilic attraction forces result in "small pores filled with liquid water and large pores covered by water film," whereas organic matter shows no water presence due to hydrophobic repulsion forces. Different water saturation levels significantly affect the relationship between pore-throat configuration and organic pore distribution, impacting effective flow pathways. The initial water saturation in shale

gas reservoirs restricts methane adsorption solely to organic pore surfaces, substantially reducing available methane adsorption sites. Particularly in continental/transitional shale gas reservoirs with high clay contents, the influence of water distribution on methane adsorption needs consideration. The proposed LBM demonstrates its ability to model sorption processes within complex porous structures efficiently. This work offers critical insights into water sorption behavior in shale's nanopore systems, laying the groundwork for modeling liquid-vapor distribution in nanoporous media at the pore scale. In addition, these findings provide theoretical support for estimating gas adsorption content and reservoir numerical simulation for shale gas reservoirs.

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MS15 / **67**

Machine learning accelerated molecular simulation: Implications for oil and gas problems

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In the last few decades, deep learning (DL) has afforded solutions to macroscopic problems in petroleum engineering, but mechanistic problems at the microscale have not benefited from it. Mechanism studies have been the strong demands for the emerging projects, such as the gas storage and hydrate production, and for some problems encountered in the storage process, which are common found as the chemical interaction between injected gas and mineral, and the formation of hydrate. Emerging advances in DL technology enable solving molecular dynamics (MD) with quantum accuracy. The conventional quantum chemical method is computational expensive, whereas the classical MD method cannot guarantee high accuracy because of its empirical force field parameters. With the help of the DL force field, precision at the quantum chemistry level can be achieved in MD. Moreover, the DL force field promotes the computational speed compared with first-principles calculations. In this study, the basic knowledge of the molecular force field and deep neural network (DNN) is first introduced. Then, three representative open-source packages relevant to the DL force field are introduced. As the most common components in the development of oil and gas reservoirs, water and methane are studied from the aspects of computational efficiency and Chemical reaction respectively, providing the foundation of oil and gas researches. However, in the oil and gas problems, the complex molecular topo structures and various element types set a high challenge for the DL techniques in MD. Regarding the computational efficiency, it needs improvement via GPU and parallel accelerations to compete with classical MD. Even with such difficulties, the booming of this technique in the area of petroleum engineering can be predictable.

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MS13 / 68

Microscopic mechanism of CO2 huff-n-puff promoting shale oil mobilization in organic/inorganic nanopores

Authors: Huaisen Song[1]; Yongfei Yang[1]; Jun Yao[2]

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CO2 huff-n-puff is a potential promising approach for enhanced recovery and sequestration of CO2 in shale reservoirs. It is of great practical significance to understand the CO2 huff-n-puff mechanism from a microscopic point of view. Here, we investigate three stages of CO2 huff-n-puff promoting shale oil mobilization from organic-inorganic nanopores by molecular dynamics simulation. We show that during the adsorption process of shale oil, due to the presence of active molecules, the adsorption density and strength of shale oil on kaolinite wall are higher than kerogen, but the influence range of shale oil is smaller than kerogen. In the CO2 soaking stage, although CO2 has a desorption effect on shale oil near both sides of the wall, stripping shale oil near the inorganic surface was more effective than the kerogen surface. In addition, due to the presence of hydroxyl on the surface, when CO2 is slightly away from the equilibrium position on the surface of kaolinite, the attraction between CO2 and kaolinite will become repulsive force under the action of electrostatic force. In the CO2 puff stage, compared with the ideal model of 0 pressure, when the CO2 puff pressure is 10MPa, CO2 can effectively dissociate the “bullet head” structure of the medium component blocking the pore exit through the synergistic effect of miscible phase, viscosity reduction and swelling. Increase overall shale oil recovery by more than 37%. This work first investigates the CO2 huff-n-puff mobilization of shale oil from multiple stages, and effectively reveal the promoting effects of CO2 on different components of shale oil in each stage of huff-n-puff.

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Poster / 69

Stress Sensitivity of Fracture Permeability in Shale Oil Reservoirs under Fluid-Solid Coupling

Author: Saipeng Huang[1]

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Introduction
Natural fractures play a crucial role in serving as the primary conduits for seepage in reservoirs, particularly in shale oil reservoirs characterized by ultra-low permeability (Zou et al., 2009; Sun et al., 2023; Bai et al., 2023). Despite the acknowledged significance of these fractures, a notable gap exists in understanding the stress sensitivity of fracture permeability in shale oil reservoirs. Addressing this knowledge deficit, our approach comprehensively investigates natural fracture permeability. This encompasses a combination of mechanical and CT scanning tests, coupled with advanced numerical modeling techniques, to bridge the existing gap and enhance our understanding of fracture permeability in shale oil reservoirs.
Methodology
We conducted multi-scale CT scanning at 25 mm and 100 mm scales, followed by the establishment of a numerical model (Fig. 1a-d). The models were constructed with specific parameters: a density of 2.65 g/cm³, a tensile strength of 8.00 MPa, a compressive strength of 46.67 MPa, a Young's modulus of 1.33 GPa, and a Poisson's ratio of 0.21. The applied confining pressure during the numerical simulation varied from 2 MPa to 10 MPa. This study introduces a fully coupled simulation that accounts for the reciprocal interactions between fluids (CH4) and solids in shale, employing COMSOL Multiphysics.
Results and Discussion
The fracture permeability of the 100 mm core ranged from 2.04×10^4 μm² to 8.67×10^4 μm², while that of the 25 mm core decreased from 1.3×10^3 μm² to 5.45×10^2 μm². Remarkably, the fracture permeability of the 100 mm core was nearly ten times higher than that of the 25 mm core (Fig. 1e). Despite the substantial difference in fracture size between the two models, their permeability exhibited a similar changing trend under varying confining pressures. Additionally, the permeability demonstrated a linear decrease with increasing confining pressure, evidenced by a reduction of 2.35 and 2.39 times the initial values for the 100 mm and 25 mm shale cores, respectively. These findings suggest a consistent stress sensitivity of fracture permeability across different fracture scales. However, it is important to note that fractures with smaller scales may experience complete closure under higher confining pressures, resulting in the total loss of permeability.

Fig. 1. A detailed description of the model creation process based on CT scanning data shale cores. (a) Identifying fractures from scanned sections, (b) segmenting the data based on specific thresholds, (c) reconstructing a 3D model structure, and (d) refining appropriate grids based on the size of the structure. (e) The fracture permeability varies vs. the confining pressures.

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of the Wufeng and Longmaxi shale in the Luzhou Block Sichuan Basin, China. Front. Earth Sci., 2023, 17(1): 337–350. [3] Bai XF, Huang SP, Wang XD, et al. Microscopic analysis of natural fracture properties in organic-rich continental shale oil reservoirs: A case study from Lower Jurassic in the Sichuan Basin, China. J. Mar. Sci. Eng., 2023, 11(5): 1036.

Conference Proceedings:

MS05 / **70**

Impacts of viscous fingering on bio-methanation risks during underground hydrogen storage

Author: Gang Wang[1]

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Hydrogen (H2) can be used as an effective energy vector and is a key element in the energy transition [1]. To accommodate the significant volume of H2 involved in the future energy mix, subsurface porous media, such as saline aquifers and depleted hydrocarbon reservoirs, is increasingly promoted as a viable option for underground H2 storage [2]. However, the reliability of this form of storage is not yet proven. One of the concerns is the impacts of microbial activity on the storage performance of H2 [3]. This is because H2 is a superb electron donor and can trigger a variety of microbial metabolism [4]. For example, H2 may initiate the bio-methanation process when carbon dioxide (CO2) is used as cushion gas in the subsurface environment. This process may lead to H2 loss and the contamination of the back produced gas. On the other hand, H2 has very low viscosity and thus is susceptible to the development of viscous fingering, when being injected to displace a more viscous fluid [5]. In this numerical work, we investigated the joint impacts of bio-methanation and viscous instability on the storage and recovery performance of H2. We have performed a range of 2D vertical cross-sectional models with a very fine cell size (0.1 m) to capture the viscous fingering in detail. It has been found that the viscous instability can expand the total size of the mixing zone and thus promote H2 consumption by methanogenesis. Since the process leads to the reduction in total gas volume, the primary purpose of cushion gas injection, which is to prevent water breakthrough, can be compromised. As a comparison, a gravity-dominated operational strategy is designed to isolate and thus ascertain the role of viscous instability on the bio-methanation process. Although gravity can drive the segregation between H2 and CO2, permeability heterogeneities lead to flow dispersions and gas mixing. However, the total mixing zone is much reduced and thus the methanogenesis is suppressed. The results of this work can be used to improve the numerical simulations associated with H2 storage in subsurface porous media, including both hydrodynamic and microbiological processes. This study should also provide useful insights and definitions of "target properties"(e.g. acceptable rate of methanogenesis) for experimentalists and industry engineers involved in screening projects for subsurface H2 storage.

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MS11 / **71**

PoroFluidics: Deterministic fluid control in porous microfluidics

Authors: Zhongzheng Wang[1]; Louis Ong[2]; Yixiang Gan[3]; Jean-Michel Pereira[4]; Jun Zhang[5]; Emilie Sauret[2]; Yi-Chin Toh[2]

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Microfluidic devices with open lattice structures, equivalent to a type of porous media, allow for the manipulation of fluid transport processes while having distinct structural, mechanical, and thermal properties. However, a fundamental understanding of the design principles for the solid structure in order to achieve consistent and desired flow patterns remains a challenge, preventing its further development and wider applications. Here, through quantitative and mechanistic analyses of the behavior of multi-phase phenomena that involve gas-liquid-solid interfaces, we present a design framework for microfluidic devices containing porous architectures (referred to as *poroFluidics*) for deterministic control of multi-phase fluid transport processes. We show that the essential properties of the fluids and solid, including viscosity, interfacial tension, wettability, as well as solid manufacture resolution, can be incorporated into the design to achieve consistent flow in porous media, where the desired spatial and temporal fluid invasion sequence can be realized. Experiments and numerical simulations reveal that different preferential flow pathways can be controlled by solid geometry, flow conditions, or fluid/solid properties. Our design framework enables precise, multi-functional, and dynamic control of multi-phase transport within engineered porous media.

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MS03 / **72**

An Efficient Numerical simulation of Reactive Flow in Fractured Vuggy Carbonate Reservoirs Considering Hydro-Mechanical coupling effects

Authors: Kang Liu[1]; Zhaoqin Huang[2]

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Fractured vuggy carbonate reservoirs are one of the most important reserves in the world, which hold great importance for increasing reserves and production. However, fractured vuggy reservoir has greatly different reservoir space and flow patterns challenging low recovery. Three types of reservoir space, including matrix pores, fractures, and vugs, coexist with strong heterogeneity, and the spatial distribution scale varies from millimeter to the meter. Acidizing is a vital stimulation technique to boost production in deep fractured vuggy carbonate reservoirs since it can effectively enhance the connectivity of fractures and vugs. The real-time dynamic alterations in the volume of matrix pores, fractures, and vugs during acidification, coupled with changes in reservoir in-situ stress, signifies a multi-field coupled problem. Currently, research on hydrological-mechanical coupling processes throughout reactive flow in porous media is restricted to single-pore and fracture models, with little consideration given to the influence of pore, fracture, and vug deformation on reactive flow. This paper puts forth a set of mathematical models and numerical simulation techniques for analyzing reactive flow in fractured vuggy carbonate reservoirs while accounting for hydro-mechanical coupling effects. Validation of the model and method is achieved through a numerical example. The results show that fractures and vugs are leading in acid flow through the medium during the acidification of fractured vuggy media. Under stress conditions, fracture closure exhibits the most substantial impact on acid flow in the fracture, followed by vug deformation. Acid fluid preferentially flows via dominant channels connected by fractures and vugs, dissolving the rock.

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MS03 / **74**

Effects of cross-scale fracture surface roughness in crystalline host rocks on hydrodynamics

Author: Wenyu Zhou[1]

Co-author: Cornelius Fischer [1]

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Granite is considered a suitable host rock for a deep geological repository for radioactive waste. Since fractures are the main flow pathways for solute transport in this material, accurate and efficient calculation of solute transport and retention phenomena is essential for predictions related to the safety case of the repository. A key issue is the effect of cross-scale surface topography and

roughness on hydrodynamics such as fluid channeling and residence time. In this study, we use a fracture geometry model based on μ-CT data and apply a finite element method to reveal the influence of fracture geometry on solute transport behavior. Due to the heterogeneity of fracture shape and aperture width distribution, it is difficult to describe the fracture geometry and morphology by a single variable. In addition, the surface roughness of fracture walls exhibits cross-scale variability due to heterogeneous material composition, which hinders the application of simplifying self-affine geometry descriptions. Instead, investigating of the role of cross-scale surface roughness in solute transport modeling is a promising approach. We investigated the sensitivity of the roughness effect by systematic modification across scales using μ-CT data of granite fractures. By comparing 2.5D vs. 3D transport model results, the role of long wavelength surface constituents and fracture bending can be investigated. The solute transport modeling was performed using the finite element code COMSOL Multiphysics. We discuss the quantitative effect of long wavelength surface building blocks on the tailing of the breakthrough curves and a weakening of the Fickian behavior. The tracer concentration fields in the 2.5D models show a high sensitivity to spatial heterogeneity. The solute transport in larger half-pores is overestimated compared to 3D models. The differences between 2.5D and 3D models due to small-scale surface roughness are considerably smaller. Nevertheless, the effect of surface roughness wavelengths on the BTC tailing behavior is not simply monotonic, which is an important effect to consider when implementing roughness parameters in transport modeling. Finally, we discuss the potential application of using power spectral density (PSD) curves as a means of assessing changes in roughness on fracture surfaces. PSD curves provide a cross-scale quantification of surface topographies. We propose the implementation of PSD curves in transport models to increase their predictive capability for contaminant migration in fractures.

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Surrogate boosting models for well placement prediction during hydrogen storage in a depleted gas reservoir

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Due to the escalating levels of greenhouse gas emissions and the growing global need for energy, there is a requirement for innovative technologies to produce eco-friendly power [1]. Hydrogen (H2) stands as a sustainable energy for the future, and its incorporation into the worldwide economic framework is imperative [2]. To facilitate H2 as a low-carbon energy option, storage solutions spanning inter-seasonal periods or even longer will be necessary. This challenge can be met by storing H2 in appropriate geological formations [3]. Using depleted oil and gas reservoirs for storing H2 aims to enhance flexibility in both future supply and seasonal usage [4].

Idendtifying optimal well locations is a complex task due to various factors like geological heterogeneity, uncertainty, fluid properties, and economic costs [5]. Traditional numerical reservoir simulations, while industry standard [6, 7], are expensive as they involve simulating all possible scenarios [8]. Machine learning offers a potential solution to simplify well placement by introducing surrogate models [9]. These algorithms based on boosting models train several weak learners sequentially, focusing on incorrectly classified instances to build a powerful ensemble framework [10]. Demonstrating consistent effectiveness, boosting algorithms outperform individual weak learners [11] and are particularly beneficial for complex oil production planning datasets [12]. They adeptly manage non-linearities, interactions among features, and random variations, enhancing precision in enhancing well placement and decision-making [9].
In this study, we investigate the comparison of two boosting algorithms, serving as rapid surrogate models (named AdaBoost and LightGBM), to achieve precise well placement in the context of seasonal H2 storage within a depleted gas field in the Middle East. H2 yearly storage in our simulations follows a routine with a single injection and withdrawal phase during winter peak demand, spanning approximately 7 and 5 months, respectively. The success metric for well placement is determined by the H2 recovery factor. The training data for these boosting algorithms were derived from a reservoir simulator. The simulations were conducted in two stages: I) production from the producing wells spanning several years until the abandonment pressure is reached, and II) H2 injection/withdrawal cycle. The second stage includes three H2 injection-withdrawal cycles, which is followed by the H2 production until reaching to maximum recovery. The boosting algorithms are tested on a simulated dataset derived from advancing to the next well locations.
The implemented boosting algorithms have demonstrated effectiveness in predicting reservoir properties in the real case study. Our assessment of the efficacy of surrogate model, compared to the execution of reservoir simulations, reveals that a single numerical simulation entails significantly several order of magnitude time to calculate well-recovery factor than running each surrogate model individually. Despite their accuracy in predicting reservoir performance, numerical simulations demand significant computational resources. On the flip side, surrogate models present a quicker option, providing results more expeditiously than comprehensive numerical simulations, all while preserving acceptable accuracy. The surrogate model's excellent performance, coupled with its effective runtime, positions the surrogate model as the sensible choice for achieving the objectives of this study.

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MS10 / **77**

Pore structure evolution of low-permeability sandstone under acid treatment: a Micro-CT investigation

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The use of acid for permeability enhancement has gained popularity in mining and oil industries to enhance the recovery rate of low-permeability formations. This study employed static acid permeability enhancement tests, flooding acid permeability enhancement tests, and micro-CT scanning to investigate the mechanism of permeability enhancement and changes in pore structure during acid treatment. The extent of reaction between low-permeability sandstone samples and four different acids was evaluated by static tests, with hydrochloric and formic acids demonstrating good performance in dissolving filling minerals. Acid flooding experiments were conducted under reservoir conditions with a constant flow rate, and decreases in pressure difference between flow inlet and outlet were observed for most experiments, indicating an increase in permeability. The pressure difference was lower for hydrochloric acid compared to formic acid at the end of flooding, with permeability increases of 283% and 120%, respectively. Micro-CT scanning before and after acid permeability enhancement tests revealed changes in pores, pore throats, and coordination numbers using Avizo software. Based on micro-CT results, acid treatment led to an increase in the number of interconnected pores, pore throats, and their equivalent radii, resulting in higher permeability. The improved permeability was primarily due to the dissolution of dolomite, as identified by SEM-EDS and ICP.

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MS09 / **78**

Multiscale Generalized Network Modeling of Carbonates with Sub-Resolution Porosity

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With advances in digital rock physics, pore-scale numerical methods have been developed to estimate various petrophysical parameters based on 3D micro-CT images. However, currently pore-scale models mostly rely on segmented dry scan of the rock sample for network extraction, and the resulting network consists only of resolved pores and throats. For complex rocks such as carbonates that encompass multiple length scales, capturing pores at every scale is often not possible due to the size-resolution trade-off. In this study, we develop a multiscale generalized network model (GNM) by including sub-resolution porosity as another throat type, called micro-links, and modify the flow model by including flow through micro-links. In single-scale GNM, resolved throats are the main pore elements in the network and are divided into corners by certain discretization levels. GNM has several benefits, such as realistic representation of the pore space with the effect of throats expanding from throat center to neighboring pore centers and detailed corner description (Raeini et al. 2017). Moreover, GNM improves the physical accuracy of model predictions by formulating the 3D interfacial curvature between two phases not only in the axial plane but also in the sagittal plane (Raeini et al. 2018; Giudici et al. 2023). We employ differential imaging of brine and dry scans to characterize connectivity and quantify unresolved porosity. We obtain a porosity map containing all voxels with their sub-resolution porosities. Using the dilation algorithm developed by Foroughi et al. (2023), each microporous voxel is labeled according to its two closest pores, and then microporous voxels with the same closest pores are classified as a micro-link. Since we consider micro-links as continuous Darcy-like porous media, we use classical empirical relationships to describe flow in micro-links. We first tested our multiscale model with highly permeable Ketton limestone. We tuned our model to mimic the reported Ketton mercury injection capillary pressure (MICP) data, which exhibited a bimodal throat size distribution, one peak at larger pores is attributed to interparticle resolved pores large enough to be captured at micro-CT voxel size, and the peak at small pore size is for intraparticle micropores. And in between, there is an intermediate interval covering unresolved macropores, which are larger than micropores but are under resolution. To achieve a good match with the MICP curve, we determine the critical micro-link porosity as the boundary between different porosity regions and evaluate their saturation exponent and grain diameter values separately. After calibrating the model with measured permeability, formation factor, and MICP data, we generate a bimodal capillary pressure curve for oil drainage into initially water-wet system. Even in the early stages of drainage, we observe an increase in the relative permeability of water, contributed by unresolved porosity. In summary, our approach shows significant promise in addressing sub-resolution porosity in a less computationally costly manner using micro-links. We aim to extend our approach to other complex multiscale systems, including fuel cells, membranes, and batteries.

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Conference Proceedings:

MS08 / **79**

Non-monotonic effect of compaction on dispersion coefficient of porous medium

Author: Yang Liu[None]

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Numerous studies have shown a non-monotonic relationship between the dispersion coefficient and the degree of compaction of porous media [1, 2]. However, the mechanism responsible for the non-monotonic variations of the dispersion coefficient remains unclear, which brings difficulties and challenges for the regulation of the dispersion coefficient of porous media.
By combining the discrete element method and the pore network model, we investigate the impact of compaction on the dispersion coefficient of the porous medium. The dispersion coefficient exhibits a non-monotonic dependence on the degree of compaction, which is distinguished by the presence of three distinct regimes in the slope of the dispersion coefficient to the pressure load. The non-monotonic variation of the dispersion coefficient is attributed to the disparate effect of compaction on dispersion mechanisms. Specifically, the porous medium becomes tightly packed with increasing pressure load, reducing the effect of molecular diffusion that primarily governs at small Péclet numbers. Simultaneously, the elevated pressure load reinforces the heterogeneity of the pore structure while reducing its connectivity, leading to enhanced disorder and elevated proportion of low-velocity regions within the porous media flow, further strengthening mechanical dispersion and hold-up dispersion, respectively, which dominate under high Péclet numbers. The competition between weakened molecular diffusion and enhanced hold-up dispersion and mechanical dispersion, together with the shift in the dominance of dispersion mechanisms across various Péclet numbers, results in multiple regimes in the slope of the dispersion coefficient to the pressure load. Our study provides unique insights into the structural design and modulation of the dispersion coefficient of porous materials.
Keywords: dispersion; compaction; non-monotonic effect.
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MS06-A / 80

Aging of liquid foam in porous media

Author: Ali Salamé[1]

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One of the key stages in materials recycling is their crushing into finer elements, i.e., granular material or powder to be sorted and re-used. Those crushed granular materials can be mixed and reshaped using binders which will make it possible to reproduce solid objects with useful purposes. Mainly, the major practical difficulty in the implementation of these granular assemblies, whether recycled or not, is the dispersion of the binder at the contacts between the grains in order to produce binder bridges that will ensure the cohesion of the whole.
Complex liquid foam (liquid foam loaded with a binding component) represents a first-choice low carbon binder precursor to be pushed through the voids offered by a packing made with such grains, to give shape to the whole and to confer significant mechanical strength. This strength is expected to depend on the microstructure of the confined foam, the latter being controlled by the bubble-to-pore size ratio “r” [1]. However, as the liquid foam undergoes the so-called coarsening mechanism, which consists in the exchange of gas between the different bubbles, the size ratio increases as function of time.
Here, we study the coarsening of liquid foam confined into the porosity of granular packings. During these experiments the liquid fraction is maintained uniform in the system by appropriated rotation of the samples in order to counteract the effects of gravity (see Figure 1). We show that coarsening is faster whenever we increase the initial confinement parameter r0 at constant liquid saturation. We find the result known from the literature for which the bubbles eventually reach pore size, which marks the end of coarsening, but we also highlighted that before stopping, there exists a regime of self-accelerated coarsening. The main deviations with respect to the coarsening of unconfined foams will be presented.

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MS05 / 81

Predicting the tensile strength of sands treated via microbially induced carbonate precipitation (MICP)

Author: Gloria Castro[1]

Co-authors: Mary Anderson [1]; James Minto [1]; Grainne El Mountassir [1]; Rebecca Lunn [1]

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Microbially Induced Carbonate Precipitation MICP has been studied over the years as a promising bio-mediated alternative to enhance the mechanical performance of porous media. Multiple studies have investigated different MICP treatment techniques and their application to coarse-grained soils. Results of these works show the evolution of transmission properties (e.g., ultrasound waves and permeability) and the increase in strength measured by direct shear, Uniaxial Compressive Strength UCS, tensile and triaxial testing, among others. These analyses have enriched our understanding of the capabilities of MICP, yet there remains a lack of predictability regarding the soil strength that can be achieved with MICP treatments.

This study uses an extensive dataset of triaxial results collected from the literature alongside new experimental data to propose a model that predicts the evolution of the tensile strengths in MICP-treated sands based on the calcium carbonate content achieved and the untreated soil index properties. In this study, we first analysed the influence of multiple soil characteristics on the final mechanical strength of MICP-treated sands using data from the literature. These preliminary analyses uncovered a gap in the data on the treatment of angular sands. To fill this gap, we conducted experiments using highly angular sand in which the MICP treatment strategy was varied to obtain multiple levels of cementation. After the MICP treatments were completed, the specimens were scanned via X-ray computed tomography before and after consolidated-drained triaxial tests, giving insight into the deformation behaviour during failure. The whole dataset was then used to assess the validity of an analytical model that builds on previous analyses to predict the tensile strength of MICP-treated sands. Our model results are remarkably consistent with all published datasets. Our research provides a robust framework for predicting the mechanical enhancement of MICP-treated sands, based on the mass of calcite precipitated and the untreated soil index properties. This is a critical step towards a more reliable use of bio-mediated soil enhancement techniques.

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MS15 / **82**

Large Scale Efficient 3D Domain Transfer for Digital Images of Porous Materials using Pseudo-3D Architectures

Author: Kunning Tang[1]

Co-authors: Peyman Mostaghimi ; Yufu Niu [2]; Ryan Armstrong [3]; YingDa Wang [3]

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Characterisation of the internal 3-dimensional (3D) structure of complex porous materials has been revolutionised with deep-learned image processing and segmentation, promising second-scale scan times with hour-scale quality, and beyond-human multi-label segmentation accuracy at a fraction of the time. However, these claims are currently only true for single-sample, single-domain cases using 2D networks on 3D data, or small 3D subdomains (<10^8 voxels) on 3D networks. These limitations are fundamental to domain mismatch between trained networks and inference inputs, dimensional blindness of 2D networks on 3D data causing z-axis misalignment (the coin-stack (CS) effect), and the incompatibility between memory inefficient 3D networks and large-scale 3D data. These interconnected issues that have prevented the true application of deep learning to 3D volume data (10^{11} voxels, typical of synchrotron and nano/micro-CT imaging) are resolved in this paper. Herein, we introduce an unpaired semantically consistent pseudo-3D approach to domain transfer capable of inference on domains approaching the tera-scale. Several important domain transfer applications are exhibited and validated using pixel metrics and physical parameters, including the enhancement of the time resolution from hour-scale to minute- and second-scale of static and dynamic scans of geological rocks while maintaining the hour-scale image quality, accurate segmentation of out-of-domain nano/micro-CT images using a pretrained segmentation models of lithium-ion batteries and hydrogen fuel cells, and efficient large-scale 3D inference (10^{11} voxels) on single GPU.

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Poster / **83**

Investigation of single particle crushing characteristics considering non-spherical shape based on DEM

Author: Xiangyu Wang[1]

Co-authors: Chenmei Huang [1]; Xiaohua Ma [1]; Zhen Liu [1]; Long Liu [1]; Chenwei Liu [1]

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The evaluation of fracture construction processes hinges on the critical factors of conductivity and the validity period of artificial fractures. It is imperative not to overlook the conductivity damage resulting from the crushing of proppant particles. Being a specialized geotechnical granular material, proppant particles undergo fragmentation when the applied compressive load surpasses their bearing capacity. The smallest unit in breakage behavior, the single particle, serves as the foundation for pertinent mechanical research.
Quartz-sand proppant particles pose a challenge for classical theories due to their complex structures and irregular shapes. Existing studies often neglect the intricate structural shape of the proppant and the complex stress environment in the reservoir, opting instead for investigations based on regularly shaped particles. This study delves into the crushing behavior of irregularly shaped quartz sand single particles, determining the critical conditions of single-particle breakage through a combined approach of numerical simulation and experiments. A discrete element model (DEM) for the crushing of quartz sand single-particles under closure pressure and confining pressure was established. The analysis of crushing characteristics involves examining the dynamic distribution of the crushing belt and stress-strain curves. Additionally, the primary controlling factor influencing the crushing behavior of single particles is investigated.
The results reveal a unimodal distribution in the stress-strain curve for proppant particles. Smaller particle sizes correspond to higher effective peak values of fragmentation and smaller strains. Specifically, under consistent parameter conditions, 40–70 mesh quartz sand particles exhibit stress peaks over twice as high as those of 8–16 mesh particles. Larger particle sizes harbor a greater number of internal natural cracks and defects, thereby diminishing the particles' bearing capacity. The influence of particle sphericity on crushing patterns and crack locations is governed by the mode of contact between particles and the wall surface. Particles with high roundness are more likely to be broken into two parts. Concurrently, as particle irregularity intensifies, secondary cracks emanate within the particles prior to complete fragmentation, resulting in a stress-strain curve exhibiting a multi-peak distribution. For a consistent 8–16 mesh of quartz sand particles, the peak crushing force under conditions of high roundness surpasses that under conditions of low roundness by approximately 15 N. Notably, the crushing strain is significantly greater, nearly 10%, for small-sized particles compared to large-sized particles under conditions of low sphericity, whereas this difference diminishes to 1.8% under conditions of high sphericity. The experimental approach was used to validate the simulation results, immensely contributing to providing theoretical underpinnings for the application and optimization of proppants.

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MS12 / 85

Adsorption induced Effective Stress in Porous Media

Authors: Chao Zhang[None]; Shaojie Hu[None]; Ning Lu[None]

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Adsorption and capillarity, in the order of high free energy to low, are the two soil–water interaction mechanisms controlling the hydro-mechanical behaviour of soils. Yet most of the poroelasticity theories of soil are based on capillarity only, leading to misrepresentations of hydro-mechanical behaviour in the low free energy regime beyond vaporisation. This inability is reasoned to be caused by two major limitations in the existing theories: missing interparticle attraction energy and incomplete definition of adsorption- induced pore-water pressure. A poroelasticity theory is formulated to incorporate the two soil–water interaction mechanisms, and the transition between them –that is, condensation/vaporisation, by expanding the classical three-phase mixture system to a four-phase mixture system with adsorptive water as an additional phase. An interparticle attractive stress is identified as one of the key sources for deformation and strength of soils induced by adsorption and is implemented in the poroelasticity theory. A recent breakthrough concept of soil sorptive potential is utilised to establish the physical link between adsorption-induced pore-water pressure and matric suction. The proposed poroelasticity theory can be reduced to several previous theories when interparticle attractive stress is ignored. The new theory is used to derive the effective stress equation for variably saturated soil by identifying energy-conjugated pairs. The derived effective stress equation leads to Zhang and Lu's unified effective stress equation, and can be reduced to Bishop's effective stress equation when only the capillary mechanism is considered and to Terzaghi's effective stress equation when a saturated condition is imposed. The derived effective stress equation is experimentally validated for avariety ofsoil in the full matric suction range, substantiating the validity and accuracy of the poroelasticity theory for soil under variably saturated conditions.

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MS15 / **87**

Unsupervised resolution boosting of µCT scans integrated into a supervised convolutional network to predict 3D rock properties

Author: Saeid Sadeghnejad[1]

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The anticipation of fluid transport behavior within porous media holds significant importance in a diverse array of applications, encompassing subsurface hydrology (Hu and Pfingsten 2023); petroleum industry (Moslemipour and Sadeghnejad 2021), geothermal energy utilization (Meller et al. 2017), and secure subsurface storage of hydrogen or CO2 (Esfandi et al. 2023, Kanaani et al. 2023). Pore-scale properties can be obtained by building a reliable digital twin of porous media through the digital rock physics (DRP) workflow (Sadeghnejad et al. 2022).
Various imaging techniques, such as X-ray computed tomography (XCT), scanning electron microscopy (SEM), and focused ion beam-SEM, have been incorporated into the DRP workflow for

capturing rock properties (Sadeghnejad et al. 2021). However, they all are plagued by a well-known battle between scanning resolution and field of view (FoV). When increasing the FoV, scan resolution diminishes, making it unfeasible to obtain high-resolution scans over a large FoV (e.g., laboratory-scale), which could encompass all small-scale heterogeneities. Moreover, direct numerical simulation (DNS) approaches cannot simulate digital twins at the Darcy scale because of their demanding computational power. Consequently, alternative approaches, like integrating deep learning with DRP, offer a more efficient means of estimating rock properties.

In this study, we integrate an unsupervised resolution-boosting algorithm with a supervised convolutional network to predict rock properties from 3D low-resolution micro-CT scans. The semi-supervised approach involves two networks: an auto encoder and a convolutional neural network (CNN). The auto encoder network is trained on unlabelled low- and high-resolution 3D image pairs to enhance the resolution of low-quality images. The dataset comprises 35,680 3D scans of five distinct rock types (i.e., Berea sandstone, Edward Brown Carbonate, Fontainebleau sandstone, and Rotliegend sandstone) captured at two different resolutions. The scans are segmented with a Random Forest classifier algorithm integrated in ilastik, version 1.3.3, (Berg et al. 2019). Subsequently, the latent information from the AE network is combined with a conventional CNN to directly predict the pore-scale properties (i.e., porosity, permeability, tortuosity, and specific surface area) form the low-resolution images. To assess the prediction performance of this coupled network, we compare the predictions with the DNS approach computed by GeoDict 2023 (Math2Market GmbH, Germany) via the R-Squared evaluation metric.

This approach enables us to leverage a small amount of labelled data for the direct prediction of pore-scale properties from cost-effective, low-resolution images. When applied to the validation dataset, the AE-CNN network achieved an R-Squared value higher than that for the CNN not integrated with AE. To assess the model's generalization capability, a new scan from a distinct Berea sandstone sample, which was neither part of the training nor the validation data, was utilized as a test dataset. A noteworthy mean R-Squared increase was observed on the test dataset, when the AE-CNN network was implemented. This outcome underscores the substantial enhancement in prediction performance achieved through the integration of the semi-supervised network when working with low-resolution images of porous media.

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MS01 / **88**

Structure and Properties of 316L Sinter Paper for Use as Gas Diffusion Layer in PEM Fuel Cell Applications

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A manufacturing process derived from paper technology can be used to produce a flat porous metallic material. To this end, organic fibers, fillers and additives are mixed with metal powder and the pulp is subsequently processed on a paper making machine. The so-called green paper is then subjected to a heat treatment where the organic components are removed. After that, the remaining sheets are sintered at temperatures close to the melting point of the metal powder, resulting in a purely metallic porous material, the so-called sinter paper. This approach has been used for the development of an innovative Gas Diffusion Layer (GDL) for mobile fuel cells. GDLs are situated between the bipolar plate and the electrode inside the fuel cell stack. They ensure optimal gas distribution as well as the removal of water, heat and electricity and have therefore to comply with complex requirements with regard to electrical conductivity, mechanical properties, as well as wetting behavior and fluid flow properties.
So far, metallic sinter paper that meets the materials specification of stainless steel 316L could be made. The thickness of the paper is around 200 µm, and the porosity of the base material reaches values of approximately 60 %. A thorough morphological characterization was carried out based on high-resolution µCT scans and analyzed via the software package GeoDict. Measured and calculated values of the electrical and heat conductivity have been compared and first measurements of the electrochemical performance in a single-cell test bench have been carried out.

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MS17 / **89**

A Coupled THMC Model for Simulating In-situ Conversion process in Low-Medium Maturity Shale Oil Reservoir

Author: Zijie Wang[1]

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Continental shale oil in China is mainly of low-medium maturity, filled with heavy oil of low mobility and organic matter that unconverted. Horizontal drilling and hydraulic fracturing are insufficient to obtain economic production in such reservoir, thus in-situ heating and transform technology

should be applied. A multiphase multicomponent thermal-hydraulic-mechanical-chemical (THMC) coupling numerical model considering multistage kinetic reactions and solid-fluid mass conversion is developed to describe the decomposition of solid organic matter, cracking of heavy hydrocarbon, phase behavior and rock property evolution.
During the in-situ process, organic matter (kerogen) decomposition and heavy oil cracking happens, enhancing hydrocarbon mobility. The research focuses on the development of multiphase multicomponent THMC coupling model, with the evolution of porosity and permeability considered. The FVM is used for the space discretization of flow and heat transfer equation, and the open system geomechanics model is discretized with FEM. Then the fixed-stress split method is applied to solve the THMC coupling model. Finally, the impact of important parameters on cumulative production are analyzed.
The impact of parameters including heating temperature, kerogen concentration, well bottom hole pressure, heater pattern and initial water saturation on cumulative production is analyzed. The results are summarized as: kinetic reaction rate is controlled by temperature and different reactions take place at variety heating temperature, influencing the fluid composition; higher kerogen concentration can enhance cumulative hydrocarbon production after in-situ conversion, making it an important parameter to evaluate before production; low bottom hole pressure can extract hydrocarbon products in time to prevent from further cracking and coking; different heater pattern has impact on the ratio of energy output to energy input, and hexagon heater is the most benefit; high water saturation will enhance energy consumption to heat water and reduce the utility ratio of energy, thus dewater process is required to reduce water saturation. It can be concluded that the in-situ conversion process is feasible in low-mid maturity shale oil reservoir, during which kerogen decomposition and hydrocarbon cracking happens. Besides, the operating parameters should be investigated to make the heating process economical.
The proposed model provides an efficient tool for modeling the in-situ conversion process of low-mid maturity shale oil reservoirs. In this paper, the reservoir fluid property variation, in-situ porosity and permeability evolution, and production characteristics are illustrated, which could provide insights on heater design and well operational management. With multiple transport mechanisms and multi stage kinetic reactions incorporated, the hydrocarbon production characteristics and formation property evolution of shale reservoirs can be both accurately captured.

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Efficient Octree-based Permeability Computation in Reconstructed Multi-Scale Images from Subsurface Porous Rocks

Authors: Abolfazl Moslemipour[1]; Saeid Sadeghnejad[2]

Co-authors: Javad Razavi Nezhad [3]; Frieder Enzmann [4]; Davood Khoozan [3]; Thorsten Schäfer [5]; Michael Kersten [4]

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Understanding the properties of rocks is crucial in various porous media, especially in heterogeneous carbonate and tight sandstone rocks. Digital Rock Physics (DRP) has emerged as a valuable tool, which is grounded in imaging and computation. Techniques like industrial X-ray CT and FIB-SEM are usually used for image acquisition in DRP. However, these rocks are complex, with varied pores, making high-resolution (HR) imaging with a large field of view challenging because of a trade-off between resolution and field of view (FoV) [1, 2]. To tackle this, multi-scale image reconstruction methods are employed, capturing images at different resolutions and integrating statistical properties to create a unified multi-scale image. In our previous study, we introduced a method called the Octree CCSIM watershed-based multi-scale reconstruction method (OCWMR), which efficiently reconstructs multi-scale images using an octree structure [3]. This technique significantly reduces the time and memory required for reconstruction compared to previous methods. However, the reconstructed images often end up being quite large, demanding substantial memory and runtime for permeability calculations. To address this challenge, we propose a solution in this study. Instead of calculating permeability on a multi-scale image with small voxels, we perform the calculations on an image structured with an octree [4]. After reconstructing the multi-scale image using the octree structure, we directly compute image permeability on the same octree structure. This approach significantly reduces runtime and memory consumption. We tested our method on a Berea sandstone (BS) sample, calculating the permeability of individual unresolved clusters with small voxel sizes. Then, to calculate the permeability on the whole image, first, the permeability of the unresolved clusters are set separately and the permeability of the whole image is computed on the main image with large voxel size using GeoDict 2023 (Math2Market GmbH, Kaiserslautern, Germany). To validate the approach, the permeability calculated on the multi-scale image with the finest voxel size was used. With a runtime of 12 hr and by consuming 65 GB of memory, a permeabilty of 109 md was computed. Whereas, the permeability obtained from our approach was 105 md, which indicates the accuracy of our approach for calculating permeability using the octree structure. Moreover, the run time of our approach was 1 hr with a consumed memory of 2.4 GB, which are 12 folds faster and 27 folds less memory consumable than the values for the fine-resolution simualtions.

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Poster / **92**

Mechanism Research on Rapid Expansion of Steam Chamber Based on Nitrogen Inducing

Author: Haojun Xie[None]

Co-authors: Ben-Hua Zhang ; Guang-Huan Wu ; Shi-Ming Zhang

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For heavy oil reservoirs buried over 3000 ft, the high pressure would lead to low dryness and expansion difficulty for injected steam. Therefore, they are mostly developed by steam huff and puff, and the EOR methods such as steam flooding and SAGD cannot be used. As a results, the oil recovery could hardly reach 25%.
In order to solve this problem, a method of rapid expansion of steam chamber using nitrogen inducing is proposed based on nitrogen assisted flow experiment and reservoir numerical simulation study. Firstly, the effects of nitrogen concentration on partial pressure and dryness of steam under high temperature and high pressure were obtained by phase behavior experiment, which indicated that additive nitrogen amount of 20~40% would decrease the steam saturated vapor temperature over 54°F. Secondly, the phase distribution during the fluid flow and heat dissipation process were analyzed by pore-scale multiphase flow simulation, and the nitrogen would restrain the steam condensation process and increase the gas saturation along the flow direction. In the meantime, the core flow experiment shows that the nitrogen gas could decrease the multi-component fluid flow resistance over 84%, which can be considered as strong flow conductivity in porous media. Taking advantage of nitrogen gas inducing ability, the nitrogen pre-injection would build a fast flow channel in relatively higher permeability layer. It could also reduce the injection pressure over 260 psi and enhance the steam dryness about 0.15. Inside the fast flow channel, the follow-injected steam would reach a longer flow distance and higher saturation horizontal plane. As a results, the steam overlap around the injection well would get relatively slower due to the high flow velocity on horizontal plane. Then the gravity drainage process can heat and displace the heavy oil above the fast flow channel, and partial nitrogen gas would gather at the top of the reservoir and reduce the heat loss to the cap rock by 11% by reservoir numerical simulation evaluation.
Overall, this method can improve the thermal recovery over 19% and reduce the oil-steam ratio about 0.05, which provides a new way for economical thermal EOR in deep heavy oil reservoirs.

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MS01 / **94**

Performance Study of Underground Hydrogen Storage in a Saline Aquifer for a Prospective Hydrogen Pore Storage Site in Northeast Germany

Author: Anna-Maria Eckel[1]

Co-authors: Lea Döpp [1]; Márton Pál Farkas [1]; Maria Belén Febbo [1]; Ben Norden [1]; Tobias Björn Weisenberger [1]; Cornelia Schmidt-Hattenberger [1]; Ingo Sass [1]

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To address seasonal fluctuations in supply and demand for renewable energy, hydrogen (H_2) can be produced using excess electricity and temporarily stored in geological formations [1]. Due to their large volumes, widespread occurrence and distribution in sedimentary basins, saline aquifers have significant potential for underground hydrogen storage (UHS). However, large-scale UHS of pure H_2 in the porous subsurface has not been demonstrated yet. The Helmholtz research project GEOZeit focuses on preparatory research for the construction of a hydrogen pore storage demonstrator in a saline aquifer.

The precursor research contains numerical reservoir simulations with the reservoir software CMG GEM. It targets to assess the capability of UHS operations at the Triassic Stuttgart anticlinal formation near Ketzin, Germany. This formation is lithologically heterogeneous, consisting of mudstone and siltstone, and the reservoir sandstone varies in reservoir properties and thicknesses [2]. In the recent past, a large-scale CO_2 storage research project was successfully realised at the flank of the anticline [3]. Now, the top of this structure is explored to serve as a structural trap for storing H_2. However, seismic surveys revealed the presence of a fault zone at the top [2,4], indicating possible migration pathways for the gas. To study fluid flow across the fault system, different fault leakage scenarios are carried out by adjusting fault transmissibility to represent sealing or leaky faults.
To access areas situated at an increased distance from the fault zone, we are exploring the option of horizontal directionally drilled (HDD) wells to bypass the fault zone. Although vertical drilling is acknowledged as a cost-effective method, HDD excels in exploring a wider expanse of the reservoir. Given that the performance of a storage operation is strongly dependent on the well location, orientation and integrity, the comparative gas injection and withdrawal performance of a vertical versus a horizontal well layout will be presented.

For all evaluated scenarios, crucial metrics are applied to assess the quality and effectiveness of the storage operation, such as gas purity, sweep efficiency, and cyclic efficiency. The findings from the numerical studies on UHS, encompassing both general considerations and site-specific analyses at the Ketzin site, will play a crucial role in preparing and developing a prospective hydrogen demonstrator and evaluating its feasibility.

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MS08 / **95**

Quantification of crystal surface reactivity using positron emission tomography (PET) techniques

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Predicting the migration behavior of dissolved contaminants in the pore space of rock and soil is crucial for assessing the feasibility of remediation and long term waste storage strategies.
Positron emission tomography (PET) using conservative radiotracers is an established and reliable method for investigating advective flow and diffusive flux in porous geomaterials and for validating transport models [1, 2]. However, solute transport is often significantly influenced by sorption effects. Reliable data concerning these effects are crucial for analyzing remediation processes as well as predicting desired immobilization in waste storage applications.
To understand and quantify the effects of solute-mineral surface interactions, analyses beyond breakthrough curve measurements are essential. PET techniques offer unique capabilities by providing in-situ tracer propagation and concentration data with high temporal and spatial resolution, surpassing traditional flow and lysimeter experiments.
For many materials, it is desirable to quantify both reactivity and hydrodynamic flow. The simultaneous quantification of both effects requires the use of a dual tracer system. In this presentation, we discuss the possibilities of utilizing a tracer pair consisting of ^{18}F as a reactive tracer and ^{76}Br as its conservative counterpart. This allows the prediction of spatially resolved surface reactivities as well as the evaluation of advective flow. Using different sandy sediments as model systems, we demonstrate the quantifiability of localized sorption effects as low as 10 pmol/mm³.

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MS17 / **96**

The HiPerBorea project: permafrost modeling from the pore scale to the headwater catchment scale with open source, high performance computing tools

Authors: Laurent Orgogozo[1]; Thibault Xavier[1]; Simon Cazaurang[1]; Oleg Pokrovsky[2]; Sergey Loiko[3]; Anatoly Prokushkin[4]; Manuel MARCOUX[5]; Michel Quintard[6]

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This presentation aims at giving an overview of the porous media related activities of the HiPerBorea project, an ANR-funded project in its 5th and last year. The objective of this project is to enable quantitative and predictive modeling of the evolution under climate change cold regions hydrosystems. Arctic and sub-arctic areas, which are highly vulnerable to global warming, are largely covered by permafrost –soil that is year-round frozen at depth. Permafrost-affected areas, which represent 25% of emerged lands of the northern hemisphere, are prone to major biogeochemical and ecological transformations due to permafrost thaw, with strong associated feed-backs on greenhouse gas cycling (degradation of previously permanently frozen organic carbon pools).[1] Permafrost thaw has also important impacts on local populations and activities, for instance by generating soil instabilities which damage infrastructures above[2]. In order to anticipate these major changes, there is a need of modelling tools of permafrost dynamics, i.e. of heat and water transfer in variably saturated and variably frozen soils. The considered porous media are constituted of four phases, the solid phase, the liquid water phase, the ice phase and the air phase. The freeze/thaw processes induce large and abrupt variations of the transfer properties of the porous media, such as hydraulic conductivity or thermal conductivity. Then the numerical resolution of this strongly coupled and non-linear problem requires fine spatial and temporal discretizations, and thus large computation times.[3] To tackle this issue, HiPerBorea develops and uses the cryohydrogeological simulator permaFoam, an OpenFOAM solver for permafrost modelling,[4],[5] aiming at quantifying the permafrost evolution under climate change at the headwater catchment scale.[6] Meanwhile, in order to assess the transfer properties of the porous media relevant to permafrost dynamics, pore-scale studies on water and heat flow are conducted using tomographical observations and direct numerical simulations as well as pore-network modelling.[7] The main outcomes of the HiPerBorea project will be presented, and open questions related to the upscaling of numerical results from the pore scale to the headwater catchment scale will be put forward. Finally, the perspective of applications of the developed approaches will be discussed.

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MS01 / **97**

Dynamic separation of CO2 from N2 using alkali-metal forms of nanosized chabazite

Authors: Sajjad Ghojavand[1]; Svetlana Mintova[2]

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Due to the rising atmospheric concentration of CO2 from human activities, the separation of CO2 from N2, commonly referred to as flue gas, has become a crucial priority.[1] There are four prevalent technologies used for CO2 capture: (i) adsorption with amine-based solvents, (ii) adsorption by nanoporous solids, (iii) cryogenic distillation, and (iv) membrane separation. Zeolites, among the materials considered for CO2 adsorption, offer the advantage of being inorganic, non-toxic substances with high thermal stability and selectivity, which can be adjusted by their framework structure and chemical composition.[1] Moreover, recent findings indicate that zeolites exhibit flexible structures.[2] This flexibility in zeolites is observable as a response to the adsorption or desorption of guest molecules. It can manifest as changes in the zeolite lattice parameters (framework dynamics) or by the relocation of extra-framework cations within zeolite pores (extra-framework dynamics).[1,2] Traditional zeolites face diffusion limitations of guest molecules through their pore networks due to their typical existence as micron-sized polycrystalline powders.[3] To overcome these limitations, various methods have been developed to increase the surface area/volume ratio. Among these approaches, nanozeolites consisting of discrete nanoparticles that result in a greater external surface area and a higher number of available active sites.[3]

We have successfully demonstrated the outstanding CO2 capture capabilities of nanosized chabazite (CHA) zeolites in various alkali forms (Na+, K+, and Cs+).[1,3,4] In this study, we initially estimated CO2 and N2 equilibrium adsorption isotherms through Grand Canonical Monte Carlo (GCMC) calculations at 298 K. Subsequently, utilizing molecular dynamics simulations, we determined the self-diffusivities of CO2 molecules at different loadings for various CHA nanocrystals. The experimental validation of dynamic CO2/N2 separation was conducted through breakthrough measurements, simulating a 17/83 (CO2/N2) mixed-component gas mixture package at 298 K (molar basis).

Based on the breakthrough results, we obtained dynamic saturation CO2 loadings of 2.48, 1.72, and 0.57 mmol g-1 for Na-CHA, K-CHA, and Cs-CHA nanosized zeolites, respectively, with CO2/N2 molar selectivity at saturation of 62, 46, and 23. Comparing the nanosized (60 nm) Cs-CHA zeolite with its micron-sized (3 μm) counterpart, we observed significantly faster CO2 breakthrough kinetics for the nanosized Cs-CHA zeolite. Ultimately, this accelerated kinetic behavior led to a remarkable over 150% improvement in dynamic CO2 removal.

In summary, different alkali forms of nanosized CHA zeolites prove to be exceptional materials for effectively separating CO2 from N2.

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MS15 / **98**

Deep Learning enhanced multiscale rock typing for digital core modeling

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Currently, there is rapid development in the approaches for constructing and utilizing digital cores. Digital Rock Physics (DRP) methods allow for quick and non-destructive acquisition of rock properties. The process of digital rock physics involves two primary stages: model construction and simulation of physical processes on the created models.

For heterogeneous reservoir rocks, the usage of DRP is not as straight forward as for high porosity sandstones. This is due to the inherent trade-off between the spatial resolution of data and the representativeness of the model size. The primary goal of this study was to establish a technique for upscaling digital core models from micro to macro scale, enabling the computation of rock properties while accounting for heterogeneities of various scales.

The upscaling procedure involved searching for correlations between tomography data of different resolutions and transforming low-resolution tomography into a multiclass model according to the found correlation. The approach of using convolutional neural networks for high-resolution tomography data was considered as the optimal algorithm for transforming low-resolution tomography into a multiclass model. The output of the neural network was an upscaled model of lower resolution than the original tomography. Each element (voxel) of the upscaled model belonged to one of several digital types of rock, whose generalized characteristics were determined based on the analysis of high-resolution tomography data.

To validate the upscaling technique we constructed a digital model of complex carbonate reservoirs based on data from multiscale microtomography. A multiclass model concept has been created and

experimented with, enabling the computation of flows in pore spaces of various scales. By incorporating diverse pore space structures as supplementary classes in the multiscale model, it is possible to preserve a substantial physical size of the model while enhancing its level of intricacy.

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Pore-scale prediction of formation damage on permeability and porosity impairment during fine migration using deep learning

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Formation damage poses a significant challenge in the oil and gas industry, negatively affecting hydrocarbon production [1]. Various mechanisms such as fines migration, clay swelling, asphaltene deposition, and pore plugging can alter the properties of porous rocks, especially at the pore scale, changing permeability and porosity [2,3]. It is crucial to accurately predict these changes at the pore scale to reduce operational costs.

The traditional formation damage analyzing methods often involve time-consuming and expensive field and laboratory studies. In recent years, Convolutional Neural Networks (CNNs) have gained attention across various fields for their capability to predict porous media properties very fast [4,5]. To overcome the limitations of traditional approaches, this study introduces a novel methodology that employs CNNs to predict the effects of formation damage, especially fine migration, on rock properties in the digital twin of a granular porous medium. A sphere packing algorithm with grain overlapping is utilized to generate the porous media with various porosity and permeability values. A Eulerian-Lagrangian computational fluid dynamic approach [3] is used to simulate fine particle migration and deposition. The output of this pore-scale model is post-deposition porosity and permeability changes of the porous media. The 2D images of the porous media is fed into the CNN and porosity/permeability changes subsequent to the deposition are implemented as the regression parameters. During the CNN evaluation, 80% of the generated images are used as training data, and the remaining 20% are used as test data.

Various formation damage scenarios can have varying effects on permeability and porosity of the porous media at the pore scale. The proposed CNN model could predict these effects with a high

degree of accuracy. Significantly, the predictions can be obtained in a fraction of a second using CNNs, specifically on an Nvidia® GeForce GTX 1080 Ti GPU with 11 GB RAM, compared to the several core-hours of CFD simulation on a 48-core Intel® Platinum 8160 CPU 21 GHz workstation. It is evident from this efficiency that CNNs have the potential to enhance the prediction and understanding of formation damage impacts on rock properties in a more time- and resource-efficient manner as opposed to the traditional modeling approaches.

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MS07 / 102

Bridging Microscale Physics to Macroscale Models in Confined Porous Media

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Tight subsurface formations and shales often act as seals for subsurface systems that are envisioned to store fluids such as CO2 and H2 as part of a transition to low-carbon economies of the future. These seals often comprise complex nano-confined systems with heterogeneous physical and chemical features. The extreme confinement and heterogeneity in such systems present difficulties in terms of scale separation in modeling efforts. We aim to address this challenge by developing a scale translation framework that bridges the dominant physics at the microscale to model systems with complex geometries featuring a host of flow regimes. The scale-translation framework uses an optimized implementation of a multi-grid lattice Boltzmann method (MG-LB), capable of simulating complex pore networks that feature wide ranges of Knudsen numbers. The simulator is optimized using hash tables, indirect addressing, and parallelization techniques, extending the reach of the simulator to large and complex domains. The modeling tool generates a dataset of flow behavior in complex porous media, which is used to train a Machine Learning model, specifically, a deep neural

network (DNN). Features of the pore networks, such as connectivity of the pore structures and pore size distributions, serve as input and the resulting DNNs estimate the transport properties in computational domains beyond the reach of the MG-LB models. The estimates will inform the macroscale properties of large-scale and heterogeneous, confined porous media.

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MS15 / 103

Deep learning for microstructure analysis of porous media from image augmentation, and multiscale fusion to image auto-segmentation

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Based on deep generative adversarial networks, we present a comprehensive framework for image multiscale fusion and multi-component auto-segmentation, which aims to create a precise digital rock – a key part of Digital Rock Physics to predict the petrophysical properties of porous media. Compared to low-resolution images with a large field of view (FoV), high-resolution (HR) rock images are limited in number and FoV. Thus, we first use a Style generative adversarial network (StyleGAN) to augment LR images. Then, a Cycle-consistent GAN (CycleGAN) is subsequently used to fuse multiresolution images to overcome the inherent trade-off between image resolution and field-of-view, using the unpaired real-world LR/HR images and augmented HR data. It is an efficient approach to enhance LR images over large FoV and reconstruct a 3D multiscale model, eliminating the limitation of super-resolution (SR) relying on paired images. Both HR image augmentation and multiscale fusion are conducted over greyscale images. Consequently, we trained a pix2pix network to realize multi-component auto-segmentation based on the labelled images artificially segmented into multiple minerals, along with their corresponding HR images. The workflow is quantitively validated over shale images at each above-mentioned section through petrophysical properties, such as the porosity (area or volume fraction of different minerals), two-point correlation function, pore size distribution, and apparent permeability, showing that the synthetic HR images and SR images are comparable to the ground truth. The trained pix2pix network can accurately capture the spatial distribution and morphology of different minerals. The proposed workflow provides a reliable pathway to reconstruct multiscale and multi-component digital rocks with large FoV for further pore-scale microstructure properties and fluid flow mechanism estimation, in the field of underground energy development, hydrogen storage, and carbon sequestration.

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MS17 / 104

Evaluating and enhancing the fracture conductivity by an optimised carrier fluid and proppant design

Author: Duo Wang[1]

Co-authors: Jiayuan Zhang [1]; Yunong Wu [1]; Jun Feng [1]; Xiaofang Jiang ; Zhejun Pan [1]

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Despite the fact that China has become one of few countries that can achieve economic exploitation of continental shale oil and gas, we are still confront of tricky challenges in further enhancing the recovery of hydrocarbon. Among the influencing factors, the long-term fracture conductivity after hydraulic fracturing plays a crucial role in the overall productivity of the well. Meanwhile, the stimulation of natural fissures, which are expected to collaborate with the artificial fractures, is also of great significance to an improved reservoir permeability. This requires a well-projected design and injection scheme of fracturing fluids and proppant. On top of that, a better understanding of the transport mechanism of such a fluid-particle-based system at the particle-scale can promote an optimised combination of fracturing fluid and proppant.

Hence, the aims of the current research include a parametric study of the particle-laden flow in the fractures and a systematic evaluation of the conductivity of the propped fractures. The study on proppant transport is accomplished by means of numerical simulation. The implemented numerical framework consists of the lattice Boltzmann method (LBM) for the fluid and the discrete element method (DEM) for the large number of moving particles. A partially saturated boundary condition is applied to provide an accurate characterisation of the fluid-solid boundaries. The transport mechanism of the proppant at the artificial-natural fracture intersection as well as the flowback mechanism of the proppant are studied. Factors including proppant size and concentration, aperture-to-diameter ratio, injection rate and fracture inclination are investigated in detail. Specifically, the shear-thinning rheology of the immersed proppant bed is observed, which results in a nonlinear variation of proppant bedload transport with the fluid. The fracture conductivity is experimentally evaluated using the shale cores and sand proppant at the reservoir pressure. By adjusting the proppant aspect ratio, we find an optimised proppant concentration for each overburden pressure, under which the fracture conductivity reaches the maximum.

The present study can provide a powerful numerical approach towards a particle-scale characterisation of proppant transport. Besides, it also formulates an efficient workflow to evaluate and optimise both short- and long-term fracture conductivity. The outcome of the current research contributes to a better design of the fracturing fluid comprising of the carrier fluid and proppant. It also provides a theoretical basis for an optimised proppant selection for future hydraulic fracturing operations, which benefits the exploitation of the continental shale oil in China.

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MS13 / 105

Occurrence characteristics and quantitative evaluation of micro-nano pore shale oil: A case study of Lianggaoshan Formation shale strata in northeast Sichuan, China

Author: Xuefeng Bai[1]

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The reservoir space of shale series is mainly composed of micro and nano pores. It is significance to carry out the occurrence characteristics and quantitative evaluation of shale oil with micro- nano pores for the study of shale oil rich and integrated reservoirs. In 2020, Well Ping'an 1, located in the northeastern region of Sichuan Basin, achieved a high yield of 100 tons in Jurassic Lianggaoshan Formation shale, realizing a major breakthrough in shale oil and gas exploration of Lianggaoshan Formation in Sichuan Basin and showing a broad exploration prospect of shale oil in this area [1]. However, the rapid sedimentary facies change, complex and diverse lithofacies, large maturity distribution range (Ro: 0.9%-1.9%), and multiple oil types of the shale strata in the Lianggaoshan Formation lead to unclear occurrence characteristics and content of micro-nano pore shale oil, which seriously restricts the optimization of favorable zones in this area [2]. Therefore, taking the medium-high mature shale strata of Lianggaoshan Formation in northeast Sichuan area of China as an example, this study carried out experimental analysis of conventional core and preserved core samples in the study area, such as scanning electron microscopy, low-temperature nitrogen adsorption, high-pressure mercury injection, nuclear magnetic resonance, multi-step pyrolysis, and original oil and gas chromatography. The results show that oil film/carbon slag is widely developed in the micro-nano pores of shale, and the lower limit of free oil pore size is ~3nm. The occurrence (oil) volume of organic-rich layered clay shale and organic-low layered felsic shale is the largest. TOC, clay content and maturity are the main control factors of oil adsorption in Lianggaoshan shale. Combined with light hydrocarbon recovery and heavy hydrocarbon correction, the total oil content calculation model of the original formation in the study area is determined. The total oil content of the organic-rich layered clay shale and organic-low layered felsic shale is higher than that of other rock facies, which can be used as a favorable oil reservoir for research.

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The impact of dispersion on porous media gravity current propagating over an interbed layer

Author: Saeed Sheikhi[1]

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Gravity currents in porous media play a crucial role in various geophysical flows e.g. seawater intrusion in coastal aquifers, underground hydrogen storage (UHS), and CO_2 or acid gas sequestration. We therefore developed a theoretical and numerical model to study the evolution of a gravity current with a particular focus on the interaction between its bulk and dispersed phases. Our models assume that the gravity current experiences distributed basal drainage along a low-permeable interbed layer. The requirement to incorporate dispersion arises from empirical observations of miscible gravity currents undergoing drainage. Our theoretical model considers the mass exchange between the bulk and dispersed phases to include dispersion. Basal draining is modeled with reference to two book-end limiting formulations, i.e. no mixing vs. perfect mixing in the lower layer. The accuracy of these formulations is evaluated by contrasting the theoretical model predictions with the results obtained from complementary numerical simulations conducted using COMSOL.

Our findings indicate that the extent of dispersion is influenced by the inclination angle, as well as the depth and permeability of the interbed layer. We additionally discover that the theoretical model we employ provides reasonably precise predictions for the nose position until the no-mixing model anticipates a retraction of the gravity current front.

Finally, the injection phase of UHS in a depleted gas reservoir is simulated using a reservoir simulator, OpenGoSim, to study the applicability of our theoretical model to real geological layers. The results justify that the simplifying assumptions in our theoretical model do not limit its predictive accuracy.

Funding acknowledgment: NSERC

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MS06-A / 108

Multiphase Flow Behavior and Numerical Simulation in Fractured-vuggy Porous Media

Authors: Heng Zhou[1]; Zhaoqin Huang[1]

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he geological features of fractured-vuggy carbonate reservoirs are complex, primarily manifested in the multiscale nature, diverse distribution, and complex connectivity and combination of fractures and vugs. The fluid flow behavior in such media is complex, involving both porous flow in the matrix and fractures and free flow in vugs. This results in the internal flow showing features of coupled flow of two-phase or even multi-phase free flow coupling. Currently, research on the coupling of single-phase porous media flow and free flow has been very mature at home and abroad. However, the research on multiphase flow is not perfect, and the coupling mechanism is not clear, especially three-phase flow of oil, gas, and water, leading to immature development theories and methods for fractured-vuggy reservoirs and low recovery rates.As proven the behavior of three-phase flow of oil, gas, and water in fractured-vuggy reservoirs, this study, based on typical reservoir geology and flow features, designed and fabricated a physical model of fractured-vuggy media and conducted physical simulation experiments. Numerical simulation studies were then conducted based on these experiments, with the simulated flow trends being generally consistent with the experimental results. By combining numerical modeling with experimental approaches, a fundamental theoretical study on the three-phase flow of oil, gas, and water in fractured-vuggy reservoirs was conducted, illustrating the features of the three-phase flow in such media. This research has a certain guiding significance for the efficient development of fractured-vuggy reservoirs.

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A Robust three-phase equilibrium calculation framework for dimethyl ether (DME)-H2O-CO2-Hydrocarbon systems

Authors: Zhengbao Fang[1]; Hongbin Jing[1]; Huanquan Pan[1]; Jianqiao Liu[1]

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CO2 flooding is a strategic measure to enhance oil recovery (EOR) while mitigating CO2 emissions. In recent years, dimethyl ether (DME) has emerged as a promising solvent used in EOR practices. Its

potential application in CO2 flooding attracts considerable interest. However, accurate modeling of the phase behavior of the DME-H2O-CO2-Hydrocarbon system remains a challenge, which leads to the lack of a reliable reservoir simulator required by the industrial production simulation.
In this study, the phase behavior of the DME-CO2-H2O is systematically studied after the intensive literature collection and review. We developed a robust and efficient multiphase equilibrium calculation framework for the DME-H2O-CO2-Hydrocarbon systems. The Peng-Robinson EOS with the Huron-Vidal mixing rule is used as our thermodynamic model. We have implemented a combined successive substitution-Newton-trust region iterative algorithm to guarantee convergence in the stability analysis and multiphase flash calculations. Besides, the initial phase equilibrium constants (K-values) strategy is revealed to correctly detect the phase status for one-phase and two-phase stability analyses. We present the performance of our model with two characterized fluid systems from the literature. For each case, the fluid consists of 30% oil and 70% H2O, and the mixture of the different ratios of CO2 and DME is injected into the fluid. Our model works accurately and robustly for these cases, and we do not find a single mistake or convergent problem for more than tens of millions of tested points.
Our model and the developed algorithms can robustly and accurately predict the multiphase behavior of the DME-H2O-CO2-Hydrocarbon systems. To the best of our knowledge, our algorithm is the first one to meet the restricted standard for multiphase equilibrium calculations in the compositional simulation of injecting the mixture of CO2 and DME into a reservoir. Our developed method will provide the key contribution to the development of the compositional simulation for the DME-H2O-CO2-Hydrocarbon systems.

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Mechanical analysis of gas diffusion layers for PEMFCs based on orthogonal design method

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The Gas Diffusion Layer (GDL) is a critical component that ensures the efficient operation of proton exchange membrane fuel cells, capable of accommodating deformations and pressure differences between cell components. This study proposes a combined method of finite element and stochasticlly reconstruction method for GDL, calculating the stress and stress uniformity inside GDL microstructure under different compression ratios. Finally, an optimization analysis is conducted using orthogonal design method, and new stress prediction expressions are proposed. The results indicates that, fiber diameter and porosity are more sensitive. The new developped expressions are validated, which can predict and optimize the combined effects of different microstructure parameters on mechanical performance accurately. The results of this study provide predictions and guidance for designing low-stress and high-performance GDL.

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Numerical simulation and completion design optimization of sand production in depressurization exploitation of natural gas hydrate in South China Sea

Authors: Yu Qin[1]; Yiqun Zhang[1]; Xiaoya Wu[1]; Youkeren An[1]

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Natural gas hydrate has large reserves and a high level of heat value, which is the strategic commanding point of global energy development. The hydrate reservoirs in the South China Sea are shallowly buried and have low cementation strength. In the process of exploitation for the hydrate reservoirs, workers often face problems such as large sand production, formation instability, and low efficiency of exploitation. In order to further study the production capacity and sand production during the process of exploitation, this study focuses on the characteristics of hydrate reservoirs in the Shenhu area of the South China Sea. Based on the CMG-STARS platform, a numerical model, coupled with thermos-hydro-chemistry processes, was established to explore the effects of completion horizon, completion length and production pressure on reservoir productivity and sand production law in vertical well depressurization mining. The results show that: The well completion in the middle of the reservoir is 21% and 15% higher than that at the top and bottom respectively, and the cumulative gas-to-water ratio is higher and the development effect is better, while the sand production problem at the top and middle of the reservoir is more serious. Under the current simulation conditions, considering the production capacity and sand production, the exploitation effect is the best when the completion length is 10m. Continue to increase the completion length, the production increase is reduced, only 19% increase, and the sand production increases sharply. The lower the production pressure is, the better the productivity is, and the more serious the sand production is. When the production pressure continues to decrease, the yield increase effect decreases, while the sand production still increases significantly. This study can provide a theoretical basis for the development of natural gas hydrate in the South China Sea.

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MS19 / **116**

Main controlling factors and pore structure of low resistivity shale

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Abstract:The phenomenon of abnormal low resistivity values in shale is widespread at the base of the Longmaxi Formation in the southern Sichuan region,and the gas content between different low resistivity shale gas wells have obvious differences.In order to explore the controlling factors and the differences in nanoscale pore structures of different resistivity shale, the shale of the Longmaxi Formation in the Changning area of the Sichuan Basin was taken as the research object.Firstly,according to the characteristics of electric logging curves and the production capacity,the shale wells of Longmaxi Formation in Changning area were divided into ultra-low resistivity wells(Rt<1Ω·m),low resistivity wells(1Ω·m<Rt<20Ω·m),and normal resistivity wells (Rt>20Ω·m).Secondly,the effects of organic matter,conductive minerals and pore fluids on the resistivity of shale were analyzed through the rock electrical experimental,and the main controlling factors of shale resistivity were clarified.Finally, the reservoir space of the shale reservoirs of the Longmaxi Formation in the study area was characterized by argon ion polishing scanning electron microscopy, low-field nuclear magnetic resonance,carbon dioxide and nitrogen adsorption.The results show that the ultra-low resistivity wells are mainly affected by the graphitization of organic matter,which leads to the exponential decrease of shale resistivity,while the low resistivity wells are mainly affected by the high water saturation,and the shale resistivity decreases relatively little.There are great differences in the microscopic pore structure of shale reservoirs with different resistivity.The ultra-low resistivity wells have the lowest porosity (the mean is 3.38%),and the worst inter-pore connectivity and openness (the mean hysteresis coefficient is 0.21).There was little difference between the porosity of low resistivity wells(The mean is 6.22%) and normal resistivity wells (the mean is 6.14%),and the normal resistivity wells (the mean hysteresis coefficient is 0.13) were better than those of low resistivity wells (the mean hysteresis coefficient is 0.15).

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MS09 / **117**

Digital rock reconstruction considering high stress

Author: Chunqi Wang[None]

Co-authors: Zhaoqin Huang [1]; Jun Yao [2]

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Abstract
As the development of medium and shallow oil and gas reservoirs progresses into the mid-to-late stages, the focus of petroleum exploration is shifting towards deep and ultra-deep reservoirs. Deep oil and gas reservoirs are defined as those with burial depths exceeding 4500 m, while ultra-deep reservoirs refer to those buried beyond 6000 m. These reservoirs exhibit characteristics of high stress, significantly impacting the pore structure of reservoir rocks and, consequently, influencing microscopic flow of oil and gas. Digital rocks serve as a crucial platform for simulating flow at the pore scale. However, existing methods for reconstructing digital rocks fail to account for the effects of high stress. In this study, we propose a novel method for reconstructing digital rock cores considering high stress based on the discrete element method (DEM). The first step involves transforming scanned results obtained under room temperature and pressure conditions into a DEM model. We employ the watershed algorithm to segment CT scan images, utilize spherical harmonic functions to represent particle contours, and transform them into clump particles in PFC3D. Subsequently, a DEM model is established with porosity matching that of the actual rock. The accuracy of the model is evaluated using two-point correlation and linear path correlation functions. The second step involves setting micro-mechanical for the contact constitutive model between particles, applying stress simulation calculations, and converting the results into voxel data. The third step analyzes the geometric and topological structure of pores under different stress combinations, along with the evolution of permeability. The feasibility of the proposed digital rock core reconstruction method is validated through the analysis of Bentheim sandstone as a case study.
Keywords: digital rock reconstruction; the discrete element method; high stress; pore structure
Acknowledgments
This project was jointly supported by the National Natural Science Foundation of China (Grant No. 52034010), Sinopec Science And Technology Entry Program (No. P21072-1).

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Poster / 118

Experimental Validation of Pore-Scale Models for Gas Diffusion Layers in PEMFCs

Authors: Liusheng Xiao[1]; Miaoqi Bian[1]; Yushuai Sun[1]

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Pore-scale modeling developed over the past decades has become a powerful method to evaluate the effective transport properties of porous electrodes. Experimental verification for such a method is crucial to confirm the method's validity. In this study, experimental data of gas diffusion layer (GDL) are compared with results of pore-scale modeling. GDL microstructures are scanned and

reconstructed by X-ray computed tomography. Explicit dynamic simulations based on the finite element method are performed on these reconstructed models to reveal the 3D displacement of the microstructure during compression. Over the deformed models, the effective diffusivity, thermal and electrical conductivities are then computed using a pore-scale model code. It is found that, as the compression ratio increases to 30%, the fiber displacement increases obviously with significant anisotropy, and the fibers gradually squeeze into nearby pores located in the adjacent layers inside GDL. The effective diffusivity and permeability decrease by about 15% and 35% respectively. The conductivity increases by 100% and 20% in the through-plane and in-plane direction respectively. The validated methods can support microstructure optimization and transport properties improvement for different types of porous electrodes.

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MS06-A / 119

An advanced approach for upscaling hydrogen migration in diverse saline aquifers

Author: yueyang yu[1]

Co-authors: Liehui Zhang [2]; Shaomu Wen [3]; Yuanshuang Tang [2]; Yulong Zhao [2]

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Leveraging various energy storage techniques spanning daily, weekly, and seasonal cycles offers a pathway to lower carbon dioxide emissions per energy unit. Employing renewable energy for hydrogen production, storage, and recycling emerges as a highly viable tactic to manage seasonal energy fluctuations. Deep saline aquifers provide a practical solution for extensive hydrogen storage, specifically designed to fulfill long-term storage needs. This study introduces a percolation theory-based upscaling technique to lower computational expenses when simulating H2 movement across diverse saline aquifers with varying correlation lengths. Two geological models, each with different correlation lengths, illustrate the efficacy of this method. In the model featuring a 1.2-meter correlation length, the percolation-based upscaling results in H2 saturation errors of 8.76% in the primary area and 3.7% in the sink area, reducing runtime by almost sevenfold. Similarly, in the model with a 4.0-meter correlation length, final H2 saturation errors of 10.7% in the main area and 1.27% in the sink area are achieved, decreasing runtime by nearly fivefold. To enhance the credibility of the proposed upscaling technique, parameters derived from the Brooks-Corey and van Genuchten models are fine-tuned to match experimentally obtained properties of H2-water multiphase flow. The resulting broader-scale model accurately reproduces primary permeability and H2 migration patterns, maintaining errors below 5%. Crucially, key mechanisms governing H2 movement during subterranean hydrogen storage in saline aquifers are retained in the upscaled models, enabling efficient predictions of H2 saturation beneath caprock. This research deepens our insight into the intricate

H2 migration at a smaller scale within complex geological systems and sheds light on incorporating the characteristics of small-scale capillary barriers during upscaling.

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Elastic indication of fluid patch clustering in partially saturated porous media: critical saturation model

Authors: Qiang Liu[1]; Tobias M. Müller[2]; Reza Rezaee[3]; Yanli Liu[4]; Danping Cao[5]

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Knowledge related to the relations between elastic observations and fluid state cannot be overemphasized in porous media, which is of fundamental concern for the extraction of hydrocarbons, the monitoring of carbon dioxide geological sequestration, and the underground hydrogen storage. As known from previous theoretical and experimental experience, the P-wave velocity-saturation relation for partially saturated porous media is a concretization of the effect of fluid patch evolution on elastic properties. However, the P-wave velocities are not only governed by the overall saturation, but also depend on the fluid patches and their size. The patch size variation as saturation changes is commonly ignored in modelling investigations, even though it is natural to assume that fluid patches will form larger as saturation progresses and that percolating clusters will form at some critical saturation levels. To capture the evolution of patch size with saturation implied in the velocity-saturation relations, we are inspired by percolation theory. By incorporating the connectivity of water-filled patches in the continuous random medium model, we develop a critical saturation model. We apply this critical saturation model to examine recently reported experimental measurements, specifically analyzing the patch size changes. For measurements of drainage or imbibition processes in four sandstone samples, we indeed find a clear indication of growing patch size with water saturation. The predictions of the critical saturation model are in reasonable agreement with elastic observations. Our approach enhances the interpretation accuracy of the velocity-saturation relations and lays the foundation for a profound understanding of the effects of fluid clustering on elastic properties in partially saturated porous media.

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Elastic anisotropy and influencing factors of shale in the Wufeng-Longmaxi Formation

Author: Feng yutian[1]

Co-author: Hongming Tang [1]

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Abstract: The shale of the Wufeng-Longmaxi formation in the Sichuan Basin is the preferred layer for shale gas exploration in China, and its petrophysical characteristics are the key to geological and engineering dessert prediction. However, the characteristics and impact mechanisms of its acoustic wave velocity and elastic anisotropy are currently unclear. In this paper, the Wufeng-Longmaxi shale is taken as the research object, and the P-wave and S-wave velocities of the samples are tested under the loading and unloading process of confining pressure. The stress sensitivity variation of parameters such as wave velocity, wave velocity ratio, and anisotropy is discussed. P-wave and S-wave anisotropy parameters are correlated under different pressure conditions. X-ray diffraction, casting thin sections, scanning electron microscopy, micron CT scanning, and other analytical techniques are used to explore the mechanism of stress sensitivity of elastic parameters. The research results indicate that: (1) the acoustic velocities of samples from different angles are V90°>V45°>V0°, and there is a positive correlation between the wave velocity and the confining pressure. After unloading the confining pressure, irreversible plastic deformation occurs due to the closure of some micro-fractures in the rock core, causing the wave velocity to be higher than the initial value. (2) The stress sensitivity coefficient of the P-wave (The mean is 3.00m•s-1•MPa-1) is higher than that of the S-wave(The mean is 1.23m•s-1•MPa-1), and the stress sensitivity coefficient of the compacted stage(The mean is 3.02m•s-1•MPa-1) is higher than that of the elastic stage(The mean is 1.21m•s-1•MPa-1). (3) The anisotropy of P-wave and S-wave is negatively correlated with confining pressure. When the confining pressure is loaded to 65MPa, the change rate of P-wave anisotropy coefficient is 23%, and its stress sensitivity is higher than that of S-wave anisotropy coefficient (the change rate is 13.7%). After the unloading of confining pressure, the degree of anisotropy is reduced due to the closure of some micro-fractures. The empirical formula of P-wave and S-wave anisotropy parameters under different pressures is established by linear regression, which can provide a reference for the mutual prediction. (4) The variation of wave velocity anisotropy with stress can be divided into stress and material anisotropy, which are related to the directional arrangement of micro-fractures and clay minerals, respectively. The quantitative characterization of shale anisotropy can be realized by evaluating the development degree of reservoir fractures and mineral components and provides a reference for logging interpretation, dessert prediction, and fracturing construction of shale gas reservoirs.

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Visualization study on the growth and occurrence patterns of CO2-SO2 mixed hydrates in porous media

Author: Lifu Zhang[None]

Co-authors: Zhe Wang ; Wanjun Lu

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Sealing carbon dioxide (CO2) in marine sediments in the form of hydrates presents a promising approach for mitigating greenhouse gas pollution. The captured CO2 often includes other impurity gases, such as nitrogen (N2) and sulfur dioxide (SO2). It is well-established that the release of SO2 carries adverse effects on both human health and the environment. Currently, various flue gas desulfurization methods have been developed, but few methods can simultaneously achieve flue gas desulfurization and decarbonization. Consequently, the co-injection of impurity gases with CO2 into deep-sea sediments and their utilization for hydrate storage has emerged as a promising approach. While extensive studies have explored the impact of N2 on CO2 hydrate storage, the understanding of how SO2 influences the utilization of hydrate storage for CO2 remains relatively limited. In this work, we used a 2.5D microfluidic chip to characterize the pore structure of sediments in the South China Sea. Visualization studies were conducted to examine the occurrence patterns and growth habits of CO2-SO2 mixed gas hydrates under specific hydrate zone conditions (P=9 MPa, T=284.15 K) in the South China Sea under stagnant conditions. The growth and occurrence patterns of mixed gas hydrates at the pore scale were analyzed, and quantitative Raman spectroscopy was employed to investigate changes in hydrate composition within the pore space.
The results indicate that under static conditions, the dissolution and diffusion of gas are influenced by the pore structure of porous media, leading to regional differences in dissolved gas. This discrepancy can result in density variations between fluids, inducing fluid convection. This convection can place the fluid in a slightly perturbed state, facilitating the nucleation and growth of hydrates. Hydrate growth initiates from the gas-liquid interface, the region with the most severe fluid disturbance, promoting hydrate nucleation. During the hydrate growth process, it was observed that hydrates preferentially grow along regions where aqueous solutions exist, occupying all pores containing solutions. After that, the hydrate film that penetrates the gas-liquid interface extends into the gas phase. Due to the hydrophilicity of porous media and the high solubility of CO2-SO2 gas mixtures, the occurrence mode of mixed hydrates in the aqueous phase is typically patchy, while in the gas phase, it manifests as a mixed mode of pore-filling and load-bearing. Disparities in substance composition of dissolved substances in porous media were identified, with natural hydrate formation tending to occur in areas with higher local SO2 concentrations. Given the easier formation of SO2 hydrates compared to CO2 hydrates, the accumulation of SO2 in the fluid promotes the nucleation of mixed gas hydrates, where SO2 plays a crucial role in hydrate nucleation sites. Moreover, as SO2 is a polar molecule, its enhanced hydrophilic properties significantly improve the stability of CO2 hydrates, allowing them to remain stable and grow outside the stable domain. These findings contribute to a better understanding of the occurrence and growth mechanism of CO2-SO2 mixed hydrates in sediment pores, demonstrating the potential application of using hydrates to seal CO2-SO2.

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MS01 / 123

Pore-scale Diffusive Mixing Between Hydrogen and Carbon Dioxide: Implications for Underground Hydrogen Storage

Authors: Zhe Wang[1]; Yuhang Wang[2]; Huirong Guo[2]; Wanjun Lu[1]

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Underground hydrogen storage (UHS) is recognized as a viable solution for storing significant amounts of hydrogen (H2) in the advancement of a low carbon energy system. The diffusive mixing between H2 and cushion gas, which leads to a reduction in the purity of produced H2, persists through the entire storage period. Therefore, it is crucial to understand the diffusive mass transfer and its impact on the migration of H2. Due to experimental challenges, there is limited research dedicated to quantifying the diffusion between H2 and cushion gas under reservoir conditions. For the first time, we measured the diffusive process between H2 and CO2 (acting as the cushion gas) in a high-pressure capillary cell in situ. The time-dependent Raman spectroscopy was used to monitor the diffusive mass transfer, and the diffusion coefficient was determined based on the measured concentration profiles. We showed that the diffusive process was adequately captured by the Fick's second law with a constant diffusion coefficient. The diffusion coefficient scales linearly with the reciprocal viscosity of CO2 across the pressure and temperature range associated with subsurface storage conditions. Based on the measured diffusion coefficient, we quantified the diffusion distance for the mixing occurring at field-scale. Results indicate that the mixing between H2 and CO2 can reach tens of meters over a one-year period. This suggests that the dispersive mixing plays a role in the purity of produced H2.

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MS01 / 124

Pore-scale simulation of H2-brine system relevant for underground hydrogen storage: A lattice Boltzmann Investigation

Authors: Yuhang Wang[1]; Thejas Chakrapani[2]; Zhang Wen[1]; Hadi Hajibeygi[3]

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Underground hydrogen (H2) storage in saline aquifers is a viable solution for large-scale H2 storage. Due to its remarkably low viscosity and density, the flow of H2 within saline aquifers exhibits strong instability. Therefore, it is crucial to understand the flow processes of H2 and brine at the pore-scale, which can be translated into constitutive relations at continuum-scale to guide field-operations. For the first time, we develop a lattice Boltzmann model tailored for pore-scale simulations of the H2-brine system under typical subsurface storage conditions. The model captures the significant contrast of fluid properties between H2 and brine, and it offers the flexibility to adjust the contact angle to suit varying wetting conditions. The developed model is employed to investigate the pore-scale dynamics of two-phase flow composed of H2 and brine. We show that the snap-off is enhanced in a system with a higher capillary number and a smaller contact angle. These conditions lead to a reduced connectivity of the gas phase, which is unfavorable for H2 production from the aquifer. Moreover, the relative permeability curves, computed from the simulation results, exhibit distinct behaviors for H2 and brine. In the case of the wetting phase, the relative permeability can be quantified solely using the phase saturation, whereas for the non-wetting phase, the phase saturation and Euler number appear to contribute equally to the relative permeability. This implies that different formula, compared to the typically used saturation-based functions, should be considered for continuum-scale simulations.

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Stable unfitted finite element method for poroelasticity with weak discontinuity

Authors: Yimin Zhang[1]; Yuxin Tong[1]; Fanke Wu[1]; Yongliang Wang[1]; Zhijun Liu[2]

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The traditional finite element method requires that the mesh must match with various discontinuous, which can significantly increase the difficulty of preprocessing for hydrodynamic coupling problems with complex boundaries and material interfaces. In such case, the finite element method using unfitted mesh is obviously more advantageous, however, this method also has certain problems, for example, irregular mesh cutting may lead to ill-conditioned coefficient matrix to appear, which in turn affects the accuracy and stability of the algorithm. The ghost penalty technique was proposed

to overcome the ill-conditioning issue. Recently, an unfitted finite element was proposed for two-field poroelasticity problem, where stabilization terms based on the ghost penalty were developed. Material interfaces are even more difficult to deal with than the boundary as they require careful treatment of the weak discontinuity conditions as well as the mesh cutting stabilization. In this paper, we formulate an unfitted finite element for the poroelastic problem with both material interfaces and complex boundaries. A weak formulation based on the Nitsche's method was developed. Ghost penalty stabilization terms are designed for both sides of the elements intersected by the material interface. The performance of the proposed methodology is tested by several benchmark and practical hydraulic problems of complicated rock-soil mixtures. The numerical results demonstrate optimal convergence rates and low-level condition numbers independent of the mesh cutting.

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Poster / 126

Consideration of the effect of interlayer spatial distribution on the mechanical behaviour of porous media

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In the process of forming porous media by deposition of particles, due to factors such as deposition rate, gravity sorting effect and fragmentation of coarse particles, different structures of interlayers are usually formed, and the form of distribution of interlayers has an important effect on the stress distribution, structural strength and deformation properties of the porous media. However, existing structural parameters such as voidness, coordination number and friction angle cannot fully characterise the effect of interlayers on the structural stability and contact anisotropy of porous media under stress. In carrying out the research on the structural stability of porous media interlayer, the discrete element method is used to simulate the mechanical behaviour of particles in the process of compaction under triaxial stress servo, to reveal the mechanism of the influence of different interlayer parameters on the overall structure of the porous media, and to analyse the influence of the thickness and quantity of the interlayer on the mechanical behaviour and structural deformation of porous media according to the structural parameters of the formation of the porous media and the parameters of the interlayer particles. Based on the structural stability and stress anisotropy of porous media, the mechanical properties of the intercalation were found to have a particularly significant effect on the macroscopic strength and structural stability of porous media, taking into account the inter-particle contact force, contact direction, and peak stress correlation.

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MS03 / **128**

Numerical simulation of transport mechanisms for cyclic high-speed injection and production in fractured-vuggy underground gas storage

Authors: Ye Tian[1]; Yi Yang[1]; Huiyan Zhao[2]; Zehao Xie[1]; Yulong Zhao[1]; Liehui Zhang[1]

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Underground gas storage (UGS) exhibits various transport mechanisms due to their multi-cycle injection and production, often overlooked in numerical simulations. In fractured-vuggy UGS, certain mechanisms may have a stronger effect. L underground gas storage is crucial to China's first fractured-vuggy UGS group. A simulation study was conducted to investigate the effect of three transport mechanisms—stress sensitivity, relative permeability hysteresis, and high-speed non-Darcy effect of the fractured-vuggy UGS L during high-speed injection and production. Based on the geological model of the L UGS, the history matchings were separately conducted with and without considering transport mechanism to ensure model accuracy and elucidate the significance of transport mechanisms (as shown in Fig. 1). The multi-component fluid characterizations were implemented separately using the Peng-Robinson equation of state to perform the compositional simulation.

Our study found that stress sensitivity resulted in a 3.31% reduction in storage capacity and a 6.07% decrease in working gas volume. Relative permeability hysteresis led to a 9.05% decline in storage capacity and a 4.09% decrease in working gas volume. The high-speed non-Darcy effect only caused a 0.16% reduction in storage capacity but led to a 4.19% decrease in working gas volume. With increased injection and production cycles, the storage capacity steadily rises. After 25 cycles, there was a 3.97% increase in storage capacity. Stress sensitivity increased the capacity increment to 4.66%, while relative permeability hysteresis and high-speed non-Darcy effect raised the increment to 6.05% and 4.13%, respectively. The greater the impact of the transport mechanisms on storage capacity and working gas volume, the more significant the increase in storage capacity. However, this increase in capacity is attributed to the rise in cushion gas volume and does not reflect an increase in working gas volume. The coupling of stress sensitivity and relative permeability hysteresis resulted in a reduction of 6.51% in storage capacity and a decrease of 11.65% in working gas volume. The coupling of these two mechanisms reduced the loss in storage capacity but amplified the decline in working gas volume. We analyzed six effects resulting from the coupling of two mechanisms, as illustrated in Fig. 2. The coupling of the three mechanisms resulted in a reduction of 6.53% in storage capacity and a decrease of 13.44% in working gas volume (as shown in Fig. 3). Coupling with the high-speed non-Darcy effect had no extra coupling effect on storage capacity but led to a further decline in working gas volume. The mutual influence relationships among the three mechanisms are depicted in Fig. 4.

This study presents the utilization of compositional simulation to investigate the coupled effect of stress sensitivity, relative permeability hysteresis, and high-speed non-Darcy effect, as well as

the coupled effects of stress sensitivity with relative permeability hysteresis on the operation of fractured-vuggy UGS. It comprehensively quantifies the varying degrees of influence exerted by different transport mechanisms on the operation of UGS. The study offers guidance for optimizing operational strategies for the UGS L and other similar UGS converted from fractured-vuggy reservoirs.

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Poster / 129

Molecular Simulation of the Effect of Imidazolium-Based Ionic Liquids on the Water/Toluene Interface

Author: Salem Alshammari[None]

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Crude oil is a complex mixture of organic compounds which are conventionally categorized as saturates, aromatics, asphaltene and resins based on their polarity and solubility. Aromatics, in particular, comprise a large portion of many light, medium and heavy oils therefore it is important to understand their interfacial properties with water and surfactants in the context of enhanced oil recovery. In this work, we explore the effect of imidazolium-based ionic liquids on water/toluene interface using molecular dynamics (MD) simulation. Imidazolium ionic liquids are cationic organic compounds comprised of a heterocyclic aromatic head with a saturated aliphatic chain. The MD simulations were based on classical OPLS and SPC/E force fields with the leap-frog numerical integration scheme, 1.2 nm cut-off for Lennard-Jones potential and particle mesh Ewald summation for the electrostatic interactions. The interfacial tension (IFT) for pure water and toluene was found to be 36.09 mN/m at 300 K and 1 bar which is close to the experimental value of 35 mN/m. Adding imidazolium chloride at a surface coverage of two molecules for every square nanometer slightly reduced the IFT to 32.71 mN/m for the butyl chain. For Ionic liquids with octyl and dodecyl chains, the IFT of water/toluene has been significantly reduced by approximately a factor of 2 and 8, respectively. Calculations of the interaction energy between the two phases shows that imidazolium cations with longer chains interact more strongly with Toluene, thereby effectively reducing the IFT. Furthermore, density profiles across the axial-direction perpendicular to the interface shows that the ionic liquids with longer alkyl chain partition more toward the interface whereas the butyl imidazolium have a low surface excess and are not as surface active as the octyl and dodecyl imidazolium. Therefore, imidazolium interacts with toluene more via its alkyl chain and the association between the toluene and the imidazolium aromatic head is limited at the water/toluene interface.

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Remote hydraulic fracturing at weak interfaces

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As the most effective reservoir stimulation technique, hydraulic fracturing has been applied since the 1950s. At the same time, hydraulic fracturing can induce seismicity or result in the loss of containment of subsurface fluids due to the high injection pressure applied during its operation, leading some projects to eventual shut-down. To mitigate such adverse impacts, an alternative approach known as hydro-shearing has been promoted for some enhanced geothermal system projects, wherein the injection pressure is kept at a low level, aiming to stimulate pre-existing networks of fractures by shearing. However, the practical effectiveness of hydro shearing is yet to be proven. In this talk, we propose another alternative stimulation approach using a low-viscosity fluid. We numerically demonstrate that with low-viscosity fluid injection, we can fracture discontinuous interfaces such as grain boundaries or natural fractures without initiating fractures at the injection point. Our results indicate the possibility of engineering reservoir stimulation operations without applying high injection pressure.

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Study on the Influencing Factors of N2-Water Alternating Huff and Puff Oil Recovery in Tight Oil Reservoir

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Water huff-n-puff (WHP) is one of widely used methods to improve oil recovery for tight reservoirs. However, the poor flow-conductivity and low sweep efficiency in matrix also restrict its oil recovery performance. Herein, the N2-water alternating huff-n-puff (NWAHP) was put forward to improve oil recovery at reservoir conditions. firstly, the feasibility of which was confirmed by the comparison of NWAHP and WHP experiment. secondly, the effect on oil recovery of injection method, N2-water ratio (NWR), soak time and number of injected plugs were investigated. The results showed that the single-cycle oil recovery of NWAHP was 13.95%, which was 3.51% higher than that of WHP, and it can improve the effect of WHP very well. The N2-water injection process could delay the breakthrough of N2 during production due to the presence of water slug, resulting in a higher oil recovery than water-N2 injection. Increasing the NWR could enhance the elastic energy and sweep more oil into the matrix, but if the NWR was too high, N2 breakthrough would occur prematurely during production. Increasing the soak time could improve the diffusion distance of N2 in the core and the effect of water imbibition. Increasing the number of injected plugs could enhance the pressure during the injection process, thereby improve the swept volume of N2 and water.

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Study the mechanism of supercritical CO2 huff-n-puff on enhancing shale oil recovery

Author: Wenxiang Ge[1]

Co-authors: Long Liu [1]; Chenmei Huang [1]; Mingming Tian [2]; Chenwei Liu [1]; Hailong Zhao [1]

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Depletion recovery in shale reservoirs after fracturing suffers from a rapid decline in production and low recovery. The CO2 huff-n-puff oil production technology can effectively supplement formation energy, reduce oil-gas interfacial tension and crude oil viscosity, and improve the production of a single well. This technology has good application prospect in enhanced oil recovery of shale oil. Currently, researches on enhancing shale oil reservoir recovery by CO2 huff-n-puff primarily focus on the effects of field production parameters on recovery. However, there is limited research on the production characteristics of the degree of crude oil utilization and the effective range of CO2 under different pore sizes.
Supercritical CO2 huff-n-puff experiments were conducted to investigate the mechanism of CO2 huff-n-puff for enhanced recovery in shale reservoirs. The T2 and one-dimensional frequency coding maps before and after the huff-n-puff experiments were obtained by using nuclear magnetic resonance (NMR) technology, and the oil recovery, utilization range and porosity characteristics of shale cores were analyzed at different core permeability, huff-n-puff cycles and soaking time. A typical shale reservoir has been used to develop a mechanism model for a single well at the field scale, simulating CO2 huff-n-puff and water-CO2 alternating huff-n-puff at the field scale, studying CO2 diffusion in the reservoir, and investigating the effect of production capacity under different production parameters.
The results show that the CO2 injection volume has the most obvious effect on the CO2 huff-n-puff cumulative oil production, and the injection rate has less effect on the huff-n-puff effect under the optimal gas injection volume. By lengthening the soaking time, the distance of the injected CO2 effect from the proximal to the end of the core increased, the utilization of small pores increased significantly and there was an optimal soaking time. The increase in huff-n-puff cycles led to improved utilization of crude oil in the first half of the core, as well as increased utilization of medium and large pores, resulting in a production increase of approximately 74%. Due to capillary force, the recovery and CO2 diffusion effects near the borehole are better with supercritical water-CO2 alternating huff-n-puff than with CO2 huff-n-puff. However, water injection may drive some of the oil away from the borehole, resulting in an overall recovery effect that is not as good as that of CO2 huff-n-puff. Therefore, it is recommended to use CO2 huff-n-puff for new wells and water-CO2 alternating huff-n-puff for old wells with poor recovery. This study can serve as a reference for developing a reasonable technology plan for CO2 huff-n-puff in shale reservoirs.

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Numerical simulation CO2 sequestration in deep saline aquifers coupled with enhanced reservoir water and geothermal energy system recovery

Authors: Zehao Xie[1]; Yulong Zhao[1]; Cheng Cao[1]; Ruike Luo[1]; Shaomu Wen[2]; Yong Hu[2]; Xian Peng[3]; Zihan Zhao[3]; Liehui Zhang[1]

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Deep saline aquifers are ideal geological storage sites for CO2, containing abundant water and geothermal resources. Injecting CO2 into deep saline aquifers while simultaneously extracting reservoir water can slow down the rise in reservoir pressure, increasing the safety of storage. This approach also extracts water resources to offset the cost gap incurred during the storage process. Simultaneously, the heat in the reservoir water (geothermal energy) can be directly used for power generation and heating, further enhancing the resource utilization efficiency of deep saline aquifers. Therefore, a coordinated development approach for deep saline aquifers involving CO2 injection, water extraction, geothermal energy extraction, and carbon storage is proposed. This approach is divided into two phases: the first phase involves extracting formation water and geothermal energy during CO2 injection, and the second phase involves using CO2 as a heat medium to extract geothermal energy after depleting formation water. A numerical simulation model coupling gas-water two-phase heat flow is established to verify the advantages of this new development approach. Additionally, optimal injection methods, well pattern, and injection-production parameters for the new approach are provided.

The research results indicate that simultaneous water and geothermal extraction during CO2 injection can delay the rise in formation pressure, providing more storage space for CO2 and increasing the amount of sequestration. Continuing geothermal extraction after depleting formation water not only retrieves more heat but also further increases geological storage capacity. CO2 injection induces geochemical reactions, increasing porosity and connectivity, creating favorable conditions for sustained CO2 injection, and the extraction of formation water and geothermal energy. Intermittent injection is the optimal injection method to maximize the delay in formation pressure rise. Production wells and injection wells should be located in the same layer, with more injection wells placed in structurally lower positions. Taking the Qing 3rd member of the deep saline aquifer in the Daqing Oilfield, Jilin Province, as an example. The optimal injection parameters are an injection rate of 10,000 m3/d, an injection-production ratio of 0.8, a cyclic injection time of 3 months, and a cyclic injection-production time ratio of 1.

The new development approach provides a novel method and perspective for geological storage of CO2 in deep saline aquifers. Its aim is to establish a theoretical foundation and scientific basis for the efficient utilization of resources in deep saline aquifers. This research is of reference significance for supporting the “Dual Carbon” goals and promoting efficient resource coordination.

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Optimizing Battery State Estimation: Overcoming Computational Challenges with Hybrid Models

Authors: Hossein Mirzaee[1]; Serveh Kamrava[1]

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To ensure the safety and reliability of batteries it is critical to accurately estimate the internal state of the battery which is crucial in Battery Management Systems (BMSs). It is crucial to have methods which, aside from yielding accurate predictions, can be applied for real time estimations. However, the advanced BMSs generating accurate results are computationally intensive and time-consuming, limiting their direct application in real-time estimation. To overcome the computational demand Deep Neural Networks (DNNs) have been applied. However, to have highly accurate models, DNNs with more complex architectures should be applied. The complexity of their architecture will hinder their efficiency for online state estimation algorithms. To tackle the goal of having highly accurate predictions while being computationally efficient, we propose a BiLSTM model as a state estimator, with its hyperparameters automatically optimized using a Bayesian Optimization (BO) framework. We show that leveraging Bayesian inference enables the use of a highly accurate state estimator with a less complex DNN architecture, ensuring computational efficiency.

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MS18 / **139**

Microscale study on green remediation of non-aqueous phase liquid contamination in heterogeneous groundwater systems

Author: Xiaopu Wang[1]

Co-authors: Hailong Zhao [1]; Yan Li [2]; Tao Long [2]; Hangyu Li [1]

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The presence of non-aqueous phase liquids (NAPLs) like crude oil in groundwater systems is a major environmental concern. Conventional remediation methods often fail to remove NAPLs from low-permeable regions due to subsurface heterogeneity. Surfactants, like Tween80, are commonly used to enhance remediation; however, concerns about their toxicity and resulting secondary contamination remain. This study explored the use of a green bio-derived solvent and several other oil displacing agents for NAPL remediation. Two structurally different heterogeneous micromodels were designed and fabricated to mimic the longitudinal section of the heterogeneous regions of natural aquifers. The results indicated that the heterogeneity of porous media could significantly influence the displacement process and final results. Generally, the injection fluid preferred to flow

through the high permeable area with larger pore size and lower flow resistance, resulting less residual oil compared to the low permeable area under various experimental conditions, with an average difference in residual oil saturation of 56.76%. Besides, the bio-solvent could effectively mobilize and remove NAPL residuals from low permeable zones, improving the efficiency of remediation by 30-45%, compared with other agents. Our findings suggest that the bio-solvent is a promising, environmentally-friendly alternative chemical agent for ¬in situ NAPL remediation, offering improved efficiency and reduced secondary pollution.

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MS09 / **140**

Pore-scale prediction of CH4-CO2 competitive adsorption in nanoporous media coupling molecular simulation and machine learning acceleration

Author: Han Wang[None]

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In shale nanoscale pores, the CH4 molecular size is equivalent to the mineral molecular size, then, the non-negligible gas-solid molecular interactions lead to the existence of a large amount of adsorbed gas with low mobility, which has an important impact on shale gas production. Since the adsorption capacity of CO2 is higher than that of CH4, the injected CO2 can be adsorbed on the mineral surface and replace the adsorbed CH4, becoming an effective means to increase shale gas production and a potential way to realize CO2 geological sequestration. However, the current explanation of CH4-CO2 competitive adsorption is mainly limited to molecular simulation based on a single nanopore, the pore-scale competitive adsorption behavior in porous media with complex pore structure is still poorly understood and consumes a lot of computing resources.

In this paper, a multi-component lattice Boltzmann method coupled with molecular simulation and machine learning is proposed to accurately simulate and rapidly predict the competitive adsorption behavior of CH4-CO2 in shale kerogen and illite three-dimensional nanoporous media. Firstly, the density distribution of the miscible CH4-CO2 in kerogen and illite pores with different CO2 molar fractions is calculated by molecular simulation. Then, by fitting the molecular simulated density distribution, the CH4-solid and CO2-solid interaction force parameters in the multi-component lattice Boltzmann model are modified, and the CH4-CO2 competitive adsorption in kerogen and illite porous media is simulated based on the fitting parameters. Finally, the porous media are divided into 2095 pore structures by watershed segmentation algorithm, then, the artificial neural network

is trained by pore-structure characteristics and competitive adsorption capacity to accurately predict the CH4-CO2 competitive adsorption content in arbitrary pore structure and porous media.

This method overcomes the limitation of computing resource consumption of molecular and pore-scale simulations, and provides an effective method for the accurate simulation and rapid prediction of multi-phase multi-component competitive adsorption behaviors in nanoscale space.
Keywords: CH4-CO2 competitive adsorption; three-dimensional nanoporous media; lattice Boltzmann method; molecular simulation; machine learning

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Thermodynamics and Morphology of Ganglia in 2D Heterogeneous Porous Media

Author: Chuanxi Wang[1]

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Ganglia (bubbles, or droplets) are widespread in porous media of various industrial applications. Thermodynamic properties of a ganglion, including its volume (V), surface free energy (F), and capillary pressure (P_c), play pivotal roles in determining its transport and reactive performance. Although these properties in homogeneous porous media have been recently resolved [1, 2], quantitatively description of ganglia in heterogeneous media remains a challenge [3-5].

In this study, we develop a pore-scale algorithm for determining the morphologies and thermodynamic properties of hydrostatic ganglia in heterogeneous porous media (a 2D pillar array, as illustrated in Figure 1a). Notably, we reveal novel ganglion morphologies: the fluid-fluid interface can emerge between non-adjacent solid particles that do not share a pore unit (referred to as the "cross-pore interface"), although it has long been assumed that a pore is a basic unit of fluid and interface behaviors in porous media [2]. The presence of cross-pore interfaces is strongly associated with the pore-throat ratio: a smaller pore-throat ratio (wider throat) leads to a greater number of metastable

morphologies. Interestingly, these novel cross-pore interfaces can also be found in homogeneous media.

We track cycles of quasi-static growth and shrinkage of a ganglion (Figure 1b) and resolve the corresponding thermodynamic properties'evolution (Figure 1c&d). During growth, the ganglion invades pore by pore, with only one major length scale (the throat) controlling P_c. In contrast, during shrinkage, the boundary of the ganglion in different pores contracts cooperatively, exhibiting multiple scales of P_c during different stages of ganglion shrinkage. In addition, although the $F-V$ correlations of both growing and shrinking ganglia are statistically linear, the surface free energy (F) of a shrinking ganglion is, in most cases, higher than that of a growing ganglion at the same V.

This work provides insights for investigating quasi-static degassing, ganglia dissolution, and ripening processes, as well as to analyze the thermodynamic stability of dispersed fluid clusters in heterogeneous porous media. In addition, we call for attention that the term "pore"may not always be a valid basic representative unit during the description of fluid and interface behaviors in porous media, as demonstrated by the presence of cross-pore interfaces.

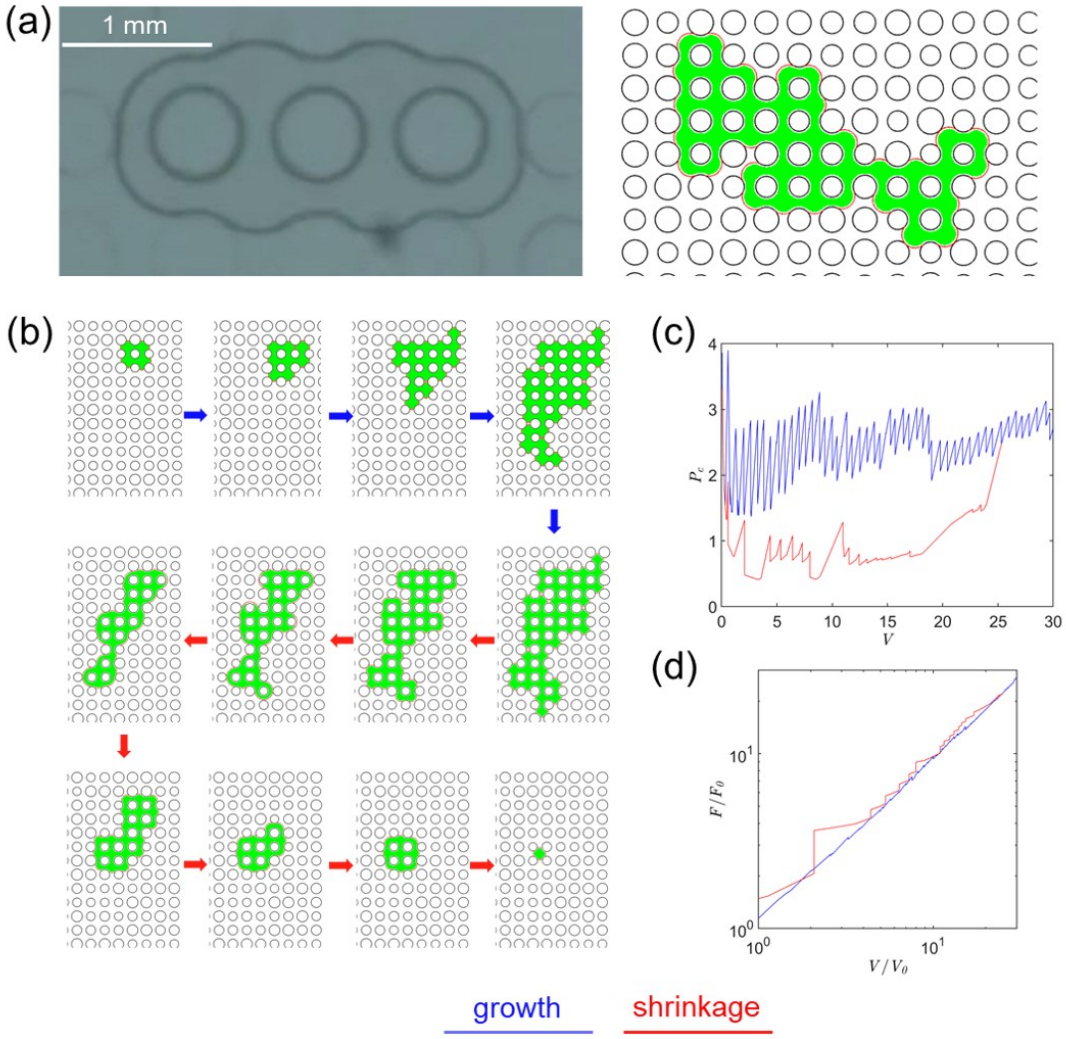

Figure 1: (a) Ganglion with cross-pore interfaces, in pore-scale experiments (left) and our model (right). (b) Snapshots of ganglion growth and shrinkage in heterogeneous porous media. (c&d) Evolution of capillary pressure (Pc) and surface free energy (F) with ganglion volume (V) during ganglion growth-shrinkage cycle in heterogeneous porous media.

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Wettability-alteration and Its Impact on Immiscible Two-phase Relative Permeability Induced by Nanoparticles Non-uniform Adsorption in Heterogeneous Porous Media

Author: Can Ke[None]

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Nanofluid injection has been reported as a promising technique to enhance oil recovery in tight reservoirs. However, research pertaining to nanoparticles (NPs) is primarily confined to laboratory experiments, thus the microscopic enhanced oil recovery mechanism behind nanofluid injection remains unclear. Therefore, it is imperative to establish a micro-scale research and analysis methodology for the nanofluid injection on macroscopic reservoir. This methodology aims to address strategically significant oilfield concerns, including: 1) NP non-uniform adsorption: The manner in which internal mineral composition, roughness, and distribution within porous media influence the non-uniform adsorption of nanoparticles, and how this non-uniform adsorption affects the microscale wettability of porous media. 2) Relative permeability: The heterogeneity in microscale wettability induced by nanoparticles and its impact on immiscible two-phase relative permeability of porous media.
In answering the question above, a novel, hybrid pore-scale simulation method using Lattice-Boltzmann (LB) coupled with Langevin-Dynamics (LD) is proposed to depict the motion behavior of NPs during immiscible two-phase displacement. In a fashion of discrete LB forcing source distribution, the LD method is introduced to characterize the effects of Brownian motion, thermal fluctuation-dissipation, and particle-particle interactions. An Eulerian-host algorithm is adopted to ensure the computational efficiency. Based on physical experimental data, NP surface properties are mathematically characterized. This coupling enables the dynamic and precise depiction of localized wettability alters within the pore-throats of reservoir. Combining with the application of statistical analysis theory, conditions governing the formation of oil-phase preferential pathways are examined, and oil/water permeabilities in tight reservoirs are calculated.
The hybrid LB-LD approach embedded experimental data and statistical analysis theory achieves the

efficient-yet-rigorous characterization of SiO2 NPs wettability alteration behaviors from representative pore-throat structures of tight oil sandstones. The results indicate: 1) Nanofluids induce a state of strong dynamic wettability heterogeneity in reservoirs by locally altering wettability. It exhibits a linear relationship with NP concentration and water-swept-area. 2) The probability density distribution of wettability in porous media exhibits a bimodal normal distribution trend. As the injection of nanofluid increases (with Sw increasing from 0.2 to 0.9), the proportion of strongly water-wet surfaces (water-wetting angle of 165°) rises from 23% to 66%, while the proportion of strongly oil-wet surfaces (water-wetting angle of 30°) decreases from 59% to 27%. 3) Quantitatively characterize the mathematical relationship between the heterogeneity in microscale wettability distribution and macroscopic permeability in porous media. Propose a probability density equation for the distribution of microscale wettability in porous media following exposure to nanofluid.
Using the method above, the microscopic mechanisms of NPs in altering wettability is examined in detail. A quantitative relationship between nanofluid injection and strong wettability heterogeneity is established, along with a clear connection between wettability heterogeneity and the reservoir permeability. The results provide important guidance not only for the prediction of micro-wettability of porous media, but also for the optimization of injection condition so that optimum oil recovery can be achieved.

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Pore-Scale Modeling of Hydrogen and Cushion Gas Relative Permeability to Brine in geological hydrogen storage

Author: Desmond Dorhjie[1]

Co-author: Alexey Cheremisin [1]

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Hydrogen is poised to become one of the most promising alternative clean sources of. energy for climate mitigation. The development of a sustainable hydrogen economy depends on the global implementation of safe and economically feasible inter-seasonal hydrogen storage and recovery. However, the current body of literature lacks a comprehensive numerical characterization of the multiphase flow of hydrogen-brine and hydrogen-cushion gas in porous media. It is crucial to study the essential parameters that impact hydrogen storage and withdrawal at the pore scale.

This study introduces a pore network model designed to replicate the underlying mechanisms of hydrogen interaction with in-situ fluids, such as brine and cushion gases. Initially, the developed pore network model is validated against laboratory measurements of hydrogen-brine drainage and

imbibition curves using the precise fluid properties and the measured petrophysical properties of the core sample. Additionally, a comprehensive sensitivity analysis was conducted to quantify the effects of fluid and rock properties on the relative permeabilities of the hydrogen phase.

The model was adapted to replicate the results of drainage and imbibition observed in the laboratory experiment of hydrogen-brine drainage and imbibition curves. Furthermore, a sensitivity analysis of the model was conducted under various conditions, including injection pressure, initial reservoir pressure, reservoir temperature, salinity of brine, and the presence of cushion gas. The results indicate that capillary pressure and the relative permeability of the hydrogen-brine system are sensitive to surface wettability. Moreover, the relative permeability endpoint (residual saturation) is significantly influenced by pore distribution and pore connectivity. A higher ratio of smaller pores correlates with a higher residual saturation of hydrogen. Conversely, the presence of a third phase (cushion gas) reduces the residual saturation of the non-wetting phase (hydrogen). Additional analysis of different cushion gases revealed that CH4 performs better as a cushion gas compared to CO2 and N2 under the simulated conditions.

This research offers a comprehensive pore-scale prediction of the relative permeability of hydrogen and brine systems, both with and without cushion gases. The analysis provides crucial quantifications of the effects of various parameters on hydrogen production. These findings contribute to the improved selection of optimal storage sites and operational parameters for the geological storage of hydrogen and its production.

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MS03 / **146**

Characteristics of CO2 Dissolution in Fractured Saline Aquifers

Author: Xiaocong Lyu[1]

Co-authors: Junxi Xiao [1]; Huiqing Liu [1]; Jing Wang [1]

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Dissolution of CO2 in brine, one of the key mechanisms for securely storing CO2 in the subsurface, involves diffusion of CO2 into the brine and subsequent buoyancy-driven convective migration. The stable stratification along the CO2-brine interface, predominated by diffusion, stimulates the density-driven convection, resulting in an enhanced dissolution rate. In fractured porous media, the complex geometry increases the uncertainty of CO2-plume migration. Predicting the characteristics of CO2 dissolution into the resident brine in fractured saline aquifers is important to understand the potential for long-term storage. In this work, a discrete fracture-matrix model (DFM), where fractures

are explicitly characterized in the model with individual grid cells, is adopted to describe the geometry of the fractured saline aquifer. We first carry out a sensitivity study to obtain a reasonable resolution of grid discretization which can capture both the fast convective flow and converged dissolution rate with fractures. Based on the selected resolution, the properties of fractures, e.g., the permeability and aperture of fractures, are investigated to confirm their impacts on density-driven convection within an individual-fracture model. In addition, an aquifer containing a complicated fracture network that includes highly intersected/dead-end fractures is used to highlight the effects of fractures on the interactions between gravity currents and convective dissolution. Our simulation results demonstrate that due to a low porosity/permeability matrix, CO2 dissolution is driven by diffusive/convection transport along the CO2-brine interface, while the density-driven convection is very weak, i.e., relatively long onset time with a small Rayleigh number. The directions of fractures play a critical role in the convective behavior of CO2-enriched brine. The fracture network enhances CO2 dissolution compared to the case of an aquifer containing isolated fractures, i.e., no connections among fractures. These estimates of the dissolution rate with fractures show that the geometry of fractures plays an important role in enhancing storage security.

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Bypass flow of trapped droplet under seismic stimulations through pore double model analysis

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Co-author: Shilin Yu [1]

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The study of trapping and releasing nonwetting droplets in porous materials has been extensively explored. However, dynamically characterizing residual nonwetting droplets under vibrations within porous media remains a challenging endeavor. Current theoretical models addressing seismic responses in two-phase flow primarily focus on single-channel geometries with fixed pressure differentials across inlet and outlet boundaries. In practical porous media, trapped droplets exist amidst flowing aqueous phases. External vibrations can induce significant pressure fluctuations due to surrounding flows, making the fixed pressure differential assumption invalid in a single-channel model. To overcome these constraints, this study delves into the micro-scale dynamics, aiming to surpass the limitations of the single-channel model. A theoretical framework involving a pore doublet, i.e., a sinusoidally constricted channel paralleled with a straight channel, is proposed to account for bypass flow effects. Initially, we analyze alterations in pressure differentials upstream and downstream of residual nonwetting droplets, considering flow dynamics during seismic excitation. We evaluate the

impact of these pressure differential variations on predictive accuracy compared to the fixed pressure differential assumption in the single-channel model. Employing the pore doublet theoretical model, we examine how the permeability of parallel straight channels influences the dynamic response of residual nonwetting droplets. Furthermore, we compare predictive discrepancies between the single-channel and pore doublet models, integrating bypass flow, to determine critical acceleration amplitudes for releasing residual nonwetting droplets at different frequencies. Ultimately, we uncover the competitive interaction between the seismic response of residual nonwetting droplets at pore throats and bypass flow in surrounding pores. These research findings establish a robust theoretical foundation for comprehending seismic impacts on engineering, geological implications, and the potential incubation of geological disasters within the geological and environmental domains.

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MS09 / 148

Theory of nonwetting fluid snap-off in porous media under vibration

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Snap-off represents a fundamental occurrence within the complex dynamics of multiphase flow in porous materials. Understanding the quantitative aspects of phenomena triggered by seismic activity within these media is vital for engineering applications and predicting natural events, particularly concerning snap-off investigations. Exploring the influence of vibrations on snap-off through numerical simulations demands substantial computational resources. Consequently, there is an urgent necessity for a theoretical model to deeply comprehend snap-off under vibrational influence. We developed a theoretical model based on volume conservation principles, elucidating the dynamic instability at the wetting/non-wetting interface in sinusoidally constricted capillary tubes experiencing vibrations. Our analysis focused on correlating vibration amplitude and frequency with non-wetting phase snap-off occurrences. Furthermore, we examined how vibrations affected nonwetting droplets, verifying adherence to static snap-off criteria. Investigating various capillaries with differing pore throat/pore size ratios allowed us to gauge the impact of vibration on snap-off. This research significantly advances our comprehension of snap-off phenomena in multiphase porous media subjected to seismic conditions, bridging a crucial gap in vibration-influenced porous media studies.

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MS13 / 149

Anomalous phase transition behavior of dilute electrolyte solutions in nanoconfinement under cryogenic environment

Author: Shaoheng Wang[1]

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The impact of confined spaces on the phase transition of water or electrolyte solutions has garnered considerable interest due to their widespread occurrence in natural processes and technological applications. [1-3] Specifically, phenomena such as freezing, melting, and vapor condensation have been extensively studied. Recently, there has been growing attention towards the phase transition of aqueous solutions, as they represent situations closer to natural and realistic scenarios than pure water.[4-5]

Notably, electrolyte solutions exhibit a slight variation from pure water, wherein an ice-salt phase separation occurs at low temperatures. The phase transition starts when ice or salt precipitates and continues until the eutectic point is reached. The eutectic point, being the lowest temperature at which a liquid solution can exist, remains constant regardless of the initial molality, and decreases with decreasing pore radius.[4] Anomalous behavior in confinement arises when the initial concentration is significantly diluted. In all studies involving a dilute solution in confinement, the thermal signal of ice and salt crystallization at the eutectic point was not observed, neither in bulk nor in the pore.[3,5]

In this work, we conducted a systematic calorimeter measurement to analyze the influence of salt molality, pore filling extent, and pore size on the transition routine of CaCl2 and NaCl solution. The results indicate that in situations with fewer salts, such as smaller pores, dilute solutions, or lower filling degrees, only water freezing at the beginning is detected, and the eutectic transition is absent due to the lack of available free ions for crystallization in the pore center. Conversely, the eutectic transition could be well detected in the solution with a larger amount of salts. This may be attributed to the uneven distribution of cations and anions in pores[6]

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MS03 / **150**

Phase-field modeling of hydraulic fracture with discrete crack topology

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Fluid-driven fracturing plays a vital role in the exploitation of geo-energy sources (geothermal, gas and oil), while also posing challenges for CO2 sequestration and underground energy storage. While the variational phase-field models have shown their power in modeling the involved crack nucleation and propagation coupled with hydro processes, the diffused representation of the cracks impedes the accurate description of the fluid flow in the discrete fracture network and the interplay between the hydraulic and mechanical processes. In this work, we developed a hybrid-dimensional model to realise a staggered description of phase-field fracture in solid media and Reynolds flow in lower-dimensional cracks. This model enables the dynamic reconstruction of 2D or 3D discrete fracture networks (DFNs) based on phase-field point cloud and unconstrained discretisations for solid and fracture domain. To avoid pressure projection when using immerse boundary condition for fluid-solid interaction, a new hydro-mechanical coupling method is proposed and verified with several numerical examples. We demonstrated that this new coupling method is efficient and more favourable when faced with complex DFNs and large-scale parallel computations.

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Enhanced oil recovery through hybrid Flue Gas-Water-Alternating-Gas (WAG) injection: Investigating the impact of water salinity on Flue Gas-WAG performance

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Abstract
This research aims to evaluate the efficiency of water-alternating-gas (WAG) methods, specifically CO2 Low-Salinity Water-Alternating-Gas (CO2-LSWAG) and flue gas-LSWAG, in comparison to High-Salinity Water-Alternating-Gas (HSWAG), within a carbonate reservoir. Employing a compositional reservoir simulator (E300), the study analyzes the effectiveness of these methods and optimizes the hybrid enhanced oil recovery (EOR) technique.

Introduction
The investigation into flue gas-LSWAG injection in geo-sequestration is crucial for improving EOR efficiency while concurrently storing CO2 and mitigating environmental impacts. A comprehensive understanding of flue gas and low-salinity water behavior in the reservoir is essential for devising more effective and sustainable approaches to enhance oil recovery and facilitate CO2 storage. This research contributes to the advancement of efficient hybrid EOR technologies, thereby supporting the transition towards a low-carbon future.

Methodology
The research employs a compositional reservoir simulator (E300) to explore hybrid EOR methods in fractured carbonate reservoirs. The model incorporates three phases: oil, gas, and water, assuming no mass transfer between water and the other phases, considering both gaseous and liquid states of the hydrocarbon mixture. The simulation process encompasses three steps. Firstly, the PVTi module simulates the reservoir fluid using oil component data. Subsequently, Eclipse software simulates flow in oil reservoir, assessing the impact of injected gas on oil recovery and the performance of conventional EOR methods. The outcomes of natural oil production are then evaluated. In the third step, various hybrid EOR methods (CO2-WAG, CO2-LSWAG, CO2-HSWAG, Flue gas-WAG, Flue gas-LSWAG, and Flue gas-HSWAG) are implemented and compared against Flue gas and CO2 injection. Finally, the results are analyzed and optimized.

Results
Comparing oil recovery factors revealed that incorporating high salinity water in CO2-HSWAG resulted in a noteworthy 12% improvement in the recovery factor. CO2-WAG exhibited superior efficiency during the early production stages, leading to a significant increase in reservoir pressure. In contrast, the sole CO2 injection method proved three times less effective in reservoir pressure increase compared to the hybrid method. CO2-HSWAG emerged as the most effective method in managing water production, contributing to approximately 90% of water production at the end of the simulation. Flue gas-WAG injection positively impacted reservoir pressure, particularly in the early production stages. Notably, the CO2-LSWAG scenario achieved the highest recovery factor in the LSWAG method investigation, demonstrating an impressive 27% improvement compared to other scenarios, reaching a level of 70%.

Conclusion
This study underscores the potential of hybrid flue gas-WAG injection to enhance oil recovery and CO2 geo-sequestration in carbonate reservoirs. The incorporation of low-salinity water and flue gas in WAG methods exhibits promising outcomes in improving oil recovery and effectively managing water production. These findings contribute to the optimization of hybrid EOR techniques and injection strategies, offering valuable insights for low-carbon future research in this domain.

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Poster / 154

Unraveling Heat Transfer Routes in Unsaturated Soils

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Thermal conductivity is a key parameter dominating the heat transfer process in a number of engineering applications such as geothermal exploitation, borehole thermal energy storage and carbon dioxide geo-sequestration. Since soil consists of multiple phases including solid particles, gas and/or water, not only the physical properties of these phases but also the routes that they form affect the heat transfer and reflect on the value of thermal conductivity. However, the heat transfer routes have not been properly identified in existing studies, which hinders the fundamental understanding of the physical mechanisms for thermal behaviour and accurate prediction of thermal conductivity in unsaturated soils.

This work aims to identify the different types of heat transfer routes and study the contribution of each type to the effective thermal conductivity of unsaturated soils. Based on computed tomography (CT) images of five glass bead assemblies varying in degree of saturation, a series of image processing algorithms were applied to the images and identified six types of heat transfer routes: (1) particles in contact surrounded by air, (2) particles in contact surrounded by both air and water, (3) particles in contact surrounded by water, (4) separate particles connected by air, (5) separate particles connected by both water and air and (6) separate particles connected by water, respectively. In addition, the amount of each type was quantified. After reconstructing digital samples from CT images and computing their effective thermal conductivity, the contribution of each heat transfer route to the effective thermal conductivity of unsaturated soils was analysed. Results show that the contribution of types 3 and 6 increases while types 1 and 4 decrease during the increase of saturation. In addition, type 2 and 5 reach their maximum contribution when the degree of saturation is at 0.2.

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Poster / 155

Effect of co-injection of acidic impurity gas and seawater on geological sequestration of CO2 in basalt

Authors: Zhe Wang[1]; Lifu Zhang[1]; Wanjun Lu[1]

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Carbon Capture and Storage (CCS) can be realized efficiently and safely by collecting atmospheric carbon dioxide (CO2) and injecting it into basalt formations in a dissolved state by co-injection of CO2 and water. In the actual storage, the collected CO2 may also contain a variety of soluble acidic impurity gases, and co-injection of acidic impurity gases with CO2 can significantly reduce the economic cost of gas collection, but the acidic impurity gases will be reacted before CO2, and there is a possibility of inhibiting the carbonation process of the minerals. In addition, the co-injection of CO2 and water is highly efficient, but it requires high freshwater resources. For coastal areas, seawater can be used instead of freshwater to reduce the dependence on freshwater resources, but at the same time, seawater injection is also more likely to affect the process of mineral sequestration. We used transparent quartz capillary tubes to simulate the reaction process between CO2 and basalt under geological reservoir conditions, and quantitatively observed the mineral reaction process after the addition of sulfur dioxide (SO2) and sodium carbonate (Na2CO3) solutions with the help of in-situ Raman spectroscopy, so as to reveal the influence of SO2 acidic gas and carbonate solution on the sequestration process of CO2 basalt. The results show:
(1) In the system consisting of only CO2 and pure water, CO2 is dissolved into water first, and then carbonate will gradually appear on the surface of basalt particles.
(2) When SO2 is added, SO2 and CO2 are dissolved into water at the same time, but sulfate and sulfite minerals appear first on the surface of basalt particles, and carbonate rocks appear on the surface of basalt particles only after SO2 is consumed by the reaction and the process of CO2 mineral sequestration occurs.
(3) The addition of Na2CO3 significantly limits the dissolution of CO2 into the water, but does not affect the dissolution of SO2. This allows SO2 to still react with basalt, while CO2 has difficulty reacting with basalt to produce carbonate minerals. This suggests that the presence of carbonate in solution further inhibits CO2 mineralization from occurring.

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MS07 / **157**

Simulation of density-driven flow in heterogenous and fractured porous media

Author: Gabriel Wittum[1]

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The study of fractured porous media is an important and challenging problem in hydrogeology. One of the difficulties is that mathematical models have to account for heterogeneity introduced by fractures in hydrogeological media. Heterogeneity may strongly influence the physical processes taking place in these media. Moreover, the thickness of the fractures, which is usually negligible in comparison with the size of the whole domain, and the complicated geometry of fracture networks reduce essentially the efficiency of numerical methods. In order to overcome these difficulties, fractures are sometimes considered as objects of reduced dimensionality (surfaces in three dimensions), and the field equations are averaged along the fracture width.
Fractures are assumed to be thin regions of space filled with a porous material whose properties differ from those of the porous medium enclosing them. The interfaces separating the fractures from the embedding medium are assumed to be ideal. We consider two approaches:
(i) the fractures have the same dimension, d, as the embedding medium i.e. they are d-dimensional;
(ii) the fractures are considered as (d-1)-dimensional manifolds, and the equations of density-driven flow are found by averaging the d-dimensional laws over the fracture width.
We show that the second approach is a valid alternative to the first one. For this purpose, we perform numerical experiments using a finite-volume discretization for both approaches. The results obtained by the two methods are in good agreement with each other.
We derive a criterion for the validity of the simplified representation. The criterion characterises the transition of a mainly parallel flow to a rotational flow, which can not be reasonably approximated using a d-1 dimensional representation. We further present a numerical algorithm using adaptive dimensional representation.

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MS05 / **158**

Co-transport of engineered nanoparticles and bacteria in soil

Author: Rima Manik[1]

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Increasing production and wide application of engineered nanoparticles lead to their ultimate release into the environment, thereby contaminating water, air, and soil. Suspended bacteria are ubiquitous in the subsurface and can affect the transport of nanoparticles. This study investigates the fate and transport of zinc oxide nanoparticles (nZnO) in saturated soil in the presence of suspended E. coli through a coupled experimental and modelling approach. E. coli was found to enhance the transport of nZnO. However, E. coli transport was retarded in the presence of nZnO. The difference in the transport behaviour of nZnO and E. coli during the cotransport and individual transport studies is because of the competition between them in finding attachment sites on grain surfaces and also due to the formation of nZnO-E. coli heteroaggregates. The experimental results were successfully simulated using a model which accounted for nZnO and E. coli retention in soil, heteroaggregation kinetics, and heteroaggregate retention in soil.

Keywords: ZnO nanoparticles, bacteria, cotransport, modeling, soil

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Poster / **160**

A Study on Stochastic Modeling of Channelized Reservoirs Based on Reinforcement Learning

Authors: Jingzhe Li[1]; Xiufan Zhang[1]; Hanhan Yang[1]; Zhongchuang Wang[1]; Lingwen Xu[1]; Dongxing Du[1]

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Channelized reservoirs, formed by ancient river sands, play a crucial role in oil and gas reservoirs. Their subsurface nature, however, poses significant challenges in direct visualization and characterization. This paper presents a novel approach to model these reservoirs by applying Q-learning, a machine learning technique. We redefine the reservoir modeling problem within a Q-learning framework, where well locations form the state space, and the reward mechanism differentiates between channel and non-channel wells. Our method utilizes the adaptive learning ability of Q-learning to predict the channel path, aiming to maximize the cumulative reward of identifying channel wells while minimizing traversal through non-channel wells. We extend our study by conducting multiple simulations and applying the results to porous media flow field simulation, which serves to test geological uncertainties. This not only provides a deeper understanding of channelized reservoirs but also showcases the potential of machine learning techniques in analyzing large datasets for geological exploration and characterization. Comparative results with traditional stochastic walk algorithms affirm the effectiveness and accuracy of our approach, offering new insights into the modeling of porous media.

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Poster / 161

Optimization of Water Control and Oil Stabilization Scheme for Edge and Bottom Water Heavy Oil Reservoir

Author: lilong Xu[1]

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In the development process of edge and bottom water heavy oil reservoir, the existence of edge and bottom water will affect the production effect of the reservoir. Compared with conventional

oil reservoirs, edge and bottom water heavy oil reservoirs have a series of production problems, such as short oil production periods without water, rapid rise in water cut, high production cost, and low economic efficiency, resulting in generally low recovery factor. In this study, the advantages of N2, foam, CO2, and the viscosity reducer were used to give full play to their synergies through combination, the water control and oil stabilization technology of edge and bottom water heavy oil reservoir was formed to inhibit the coning of bottom water, reduce the viscosity of the oil, control the rise of water cut, and achieve the effect of improving the recovery factor. Four water control and oil stabilization schemes are designed in the paper, and the optimal water control and oil stabilization huff and puff technology scheme is identified as N2 foam + CO2 viscosity reducer + N2 through one-dimensional sand-packed tube physical simulation experiments. The results show that this scheme has the triple mechanism of N2 foam can slow down the coning of bottom water, CO2 and the viscosity reducer dissolving and energizing, the synergistic viscosity-reducing effect of deep propulsion, and N2 supplementing the formation energy, which can significantly improve the oil production, reduce the water production, and inhibit the rise of water cut. The final recovery factor reached 39.81%, an increase of 16.09 percentage points. The results of this study can provide a reference basis for the development of mining technology programs for similar blocks of edge and bottom water heavy oil reservoir after entering the high water cut period.

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MS09 / 162

Pore-scale Flow Simulation of CO2 Sequestration in Deep Shale Based on Thermal-hydro-mechanical Coupled Model

Author: Ziwei Liu[1]

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The technology of sequestering CO2 in deep shale has shown great potential due to the low permeability of shale and the high adsorption of CO2 by organic-rich characteristics. Deep shale is characterized by high-temperature and high-pressure with a significant hydro-mechanical coupling effect. The Darcy-Brinkman-Stokes method was integrated with heat transfer equations to simulate thermal-hydro-mechanical coupled single-phase steady-state flow, combined with multiphase flow equations to simulate hydro-mechanical coupled transient flow under high-temperature conditions. This study aims to reveal the effect of temperature difference between CO2 and reservoir, Reynolds number, and formation pressure on the flow process of CO2 geological storage in deep shale based on the constructed real core structure consisting of organic pore, organic matter, and

inorganic matter. The results indicate that low-temperature CO2 is conducive to giving full play to the role of convection heat transfer, improving the CO2 saturation and the swept volume of organic pores. Reynolds number has a negligible impact on the transition of convective and conduction heat transfer. At higher Reynolds numbers, CO2 flows extensively and deeply, and CO2 clusters occupy a higher proportion in organic pores. The Nusselt number is higher, and convective heat transfer is more dominant under lower confining pressure. Shallower reservoirs are favorable conditions for adsorption trapping, as their cores are subjected to slightly lower confining pressure, resulting in higher CO2 saturation in the organic matter and higher sweep rate of organic pores. Our main finding is that low-temperature CO2, a higher Reynolds number and shallower buried depth favor carbon sequestration.

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Accurate Simulation of Foam Injectivity in GeoEnergy Applications: Effect of Grid Refinement

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Foam injection can improve sweep efficiency in gas-injection processes to sequester CO2 in, and to produce hydrocarbons from, porous geological formations (Bellow, 2023, Rossen et al., 2022). Surfactant-Alternating-Gas (SAG) is the preferred injection method. Liquid injectivity is typically very poor during the SAG process, which hampers foam effectiveness overall. Conventional simulators do a poor job of assessing injectivity in SAG processes. Here we determine how refining the simulation grid, and especially the size of the injection-well grid block, alters simulated injection pressure during liquid and gas injection in SAG.
The impact of foam on the mobilities of gas and liquid is highly nonlinear, with abrupt changes in mobility upon slight changes in gas saturation in the porespace (graphical abstract, left figure). We use the widely-employed STARS foam simulator to model injectivity in a SAG process. We examine the impact of grid refinement on injectivity and well-grid-block pressure. We model a 2D 5×5 grid of equal-size blocks representing a 100 m × 100 region and three refined-grid cases, in which the central grid block is partitioned into 9, 25, and 49 equal-size blocks. We compare simulated injection pressure with that from fractional-flow theory (FFT) (Al Ayesh et al., 2017). In addition, we test the effect of the Namdar Zanganeh (NZ) correction for foam dry-out and collapse (Namdar Zanganeh et al., 2014), of neglecting the Peaceman equation and, like Sharma et al. (2017), of disallowing foam in the injector grid block.

As we refine the central grid, the peak in injection-well pressure decreases, and the peaks in pressure occur earlier for both liquid and gas injection. For gas injection, incorporating the NZ correction increases injectivity in both STARS simulations and FFT calculations, but simulations are not able to match the prediction of FFT. Gas and liquid injectivities increase if one neglects the Peaceman equation. However, gas and liquid injectivities are underestimated at early times and overestimated at later times. Neglecting foam in the injection-well grid block greatly overestimates injectivity for both gas and liquid injection, especially at later times.
The central problem in the simulators is that saturation and mobility are both treated as uniform in each grid block. Moreover, each grid block experiences saturations that should disappear within a shock front (arrows in left figure) (Rossen, 2013). In reality, complex fronts propagate outward from the injection well with time (Al Ayesh et al., 2017; Gong et al., 2019). As a result, the simulator predicts that injection pressure peaks at values up to 7 times that from FFT (right figure). Surprisingly, however, the average injection pressure over time is substantially lower than that predicted with FFT. Thus the simulator overestimates the volume injected over time if injection pressure is fixed. The excessive buildup in pressure, combined with the assumption of uniform saturation in the grid block, drives water out of the injection grid block during gas injection, and gas out during water injection. This leads to an excessive peak in pressure but overestimated injectivity over time.

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MS10 / 164

Flow field tomography identifies and quantifies pore opening and clogging in sandstones

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Fluid-rock interactions drive changes in porosity and permeability. This has important consequences for the flow field development in the complex porous material and thus controls the evolution of reactive transport processes. Important applications are in the vast field of reservoir rock alteration, e.g. by coupled dissolution and precipitation processes. While dissolution processes can cause local increases in pore space and permeability, they can also lead to pore throat blockage, which can cause formation damage due to precipitation reactions and particle retention in pore throats. Although these mechanisms are understood in principle, the direct changes in the flow field they cause are difficult to observe directly. Using positron emission tomography (PET), we show how flow field heterogeneities are quantitatively affected by the coupling of dissolution reactions and pore throat blockage by particles in a long-term experiment.

Specifically, we performed a dissolution experiment focusing on calcite cement in sandstones. While dissolution is responsible for a local increase in pore space, mobilized iron oxide and sheet silicate colloids are trapped and cause a local decrease in permeability. Direct comparison of sequences of PET-derived flow field data reveals a pattern of flow field modification during this experiment. PET thus becomes a key analytical tool to localize and quantify pore-scale flow field changes, in addition to recent advances focused on the identification of flow channeling effects of advective flow 1and on the heterogeneity of diffusive flux in low permeability rocks [2].

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Poster / 165

Integration of Digital Core and Molecular Simulation for Research on Reservoir Mechanical Properties

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The mechanical parameters of reservoir rocks play a crucial role in the evaluation of unconventional reservoirs. However, due to time and cost constraints, conducting rock mechanics experiments on all formations is not feasible. Furthermore, conventional testing methods may not accurately characterize and test rocks with complex micro-structures, such as tight sandstones and shales, where pore-throat connectivity is intricate. Therefore, this study proposes a multi-scale coupled simulation approach for reservoir rock mechanical parameters. Firstly, digital core models were constructed through CT scans of four core samples obtained from the Shengli oilfield. The analysis of thin section observations, combined with the machine learning approach of random forest, was used to classify mineral phases in the cores, such as Feldspar, Quartz, Mica, and Calcite. These mineral phases were well distinguished within the core. Subsequently, crystal lattice models of these minerals were established at the molecular scale, and mechanical parameter simulations based on molecular modeling were performed. The finite difference method was employed to calculate the stress under various strain states, resulting in the Young's modulus and Poisson's ratio for each mineral component. At the core scale, finite element simulation of uniaxial compression tests was conducted using the mechanical parameters obtained from molecular simulations, to calculate the Young's modulus and Poisson's ratio of the entire core. The model established by this method accurately reflects the fine structure and heterogeneity of the rocks, thus improving the simulation accuracy and faithfully representing the mechanical behavior of rocks in experiments. Comparison with actual uniaxial compression test results indicates an average Young's modulus error of 2.44 GPa and an average Poisson's ratio error of 0.036, demonstrating that this simulation method effectively predicts rock mechanical properties, reduces the time and cost required for experiments, and retains the majority of the accuracy of the results obtained.

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Poster / 166

Brinkman double-layer model for flow at a free-porous interface

Authors: Jinliang Kang[1]; Moran Wang[1]

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The phenomenon of the Stokes–Darcy flow in coupled systems comprising a clear channel and a complex 3D porous medium is investigated through numerical and theoretical approaches. A quartet structure generation set (QSGS) method is used to generate random complex 3D porous structures imitating real structures in nature. Pore-scale flow simulations are performed using the Lattice

Boltzmann method, enabling detailed analysis and characterization of the interfacial flow phenomena. Four key parameters with clear physical meanings are introduced to capture essential aspects of the flow dynamics quantitatively, revealing intriguing linear relationships with the square root of permeability –a fundamental characteristic length scale dominating the phenomenon. Several existing models are examined by these parameters. A Brinkman double-layer(BDL) model is proposed to address the limitations of existing models. Compared with several classic models, the present BDL model stands out due to its simplicity, accuracy, and robustness, providing a comprehensive understanding of the complex flow behavior in the coupled system.

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MS23 / 168

Pore scale insights on multi-component multi-phase fluid transport phenomena in multi-scale shale pore-fracture system

Authors: wenhui song[1]; Masa Prodanovic[2]; Jun Yao[1]

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The heterogeneities of shale pore system are expressed in terms of the complex pore-fracture structure, different pore type and multi-scale pore size. Fluid transport mechanisms in shale nanopore space notably differ from that in conventional micro-scale porous media. Conventional core-scale multi-phase flow experiments are not applicable to shale because of the nanoscale pore size and the realistic multi-component multi-phase fluid flow patterns in shale are still unknown to a large extent. Therefore it is essential to study the pore-scale fluid transport mechanisms and establish the corresponding flow simulation method.
This work summarizes our recent study on multi-component multi-phase fluid transport mechanisms in shale by pore network modelling and level-set approach. We first constructed the multi-scale pore network model based on dual resolution scanning electron microscope images. The pore network multiphase flow model (PNMFM) in organic pore system is established considering nano-micro scale gas and water transport mechanisms. PNMFM in dual pore type (organic-inorganic) system is further proposed considering the influence of pore type and wettability on gas-water distribution. We further developed a general pore network-based three-phase thermodynamic equilibrium and transport model, which enables accurate prediction of multicomponent hydrocarbon–water transport properties in shale at different temperatures and pressures. Fluid flow in complex fracture systems near wellbore is influenced by heterogeneous fluid pathway structure, proppant distribution, and stress-induced fracture aperture change. To deal with this, we developed the physics-driven level set lattice Boltzmann method -coupled model to study multiphase flow properties in complex fractures during injected water flowback and proposed the upscaled relative permeability models of induced fracture network and hydraulic fracture with proppant.

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Poster / 169

Finite-size scaling for the connectivity, permeability, and dispersion of discrete fracture networks

Authors: Tingchang Yin[1]; Teng Man[1]; Pei Zhang[1]; Sergio Andres Galindo Torres[1]

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Translating fracture statistics to global hydraulic properties in subsurface fractured rocks is a complex but appealing task, as measuring parameters such as permeability can be prohibitively expensive. To tackle this challenge, we developed the finite-size scaling (FSS) hypothesis, drawing inspiration from percolation theory in statistical physics. We created numerous Monte Carlo iterations using our CUDA-based code, cuDFNsys, to simulate flow and transport in discrete fracture networks (DFNs). We generated a wide range of DFN scenarios with vastly different input parameters to ensure generality. We then nondimensionalized the obtained connectivity, permeability, (asymptotic) dispersion coefficients, density of fractures, domain sizes, and so on. By analyzing the dimensionless quantities, we found that the FSS hypothesis can predict connectivity, permeability, and dispersion as an invariant function of dimensionless density and domain sizes with several universal critical quantities. Furthermore, the FSS function can identify the transition point of dimensionless density, where permeability remains constant regardless of domain sizes. Around this point, the scale-dependence of permeability changes from negative to positive. Our findings provide a strong theoretical foundation for understanding the relationship between fracture attributes and field-scale hydraulic properties. This research inspires further investigation into applying the FSS function at the field scale, which will improve the information that earth scientists can obtain from fracture statistics

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MS17 / 170

Advancements in Hydraulic Fracturing Simulation Considering Complex Natural Fracture Distributions

Author: Weiwei Zhu[1]

Co-authors: Zhiqiang Chen [2]; Shengwen Qi [1]; Moran Wang [3]

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Hydraulic fracturing, involving the injection of highly pressurized liquid into a well to break up bedrock formations, is a widely employed method for stimulating unconventional reservoirs, such as shale oil, shale gas, and enhanced geothermal systems (Gandossi & Von Estorff, 2013). Natural fractures play a crucial role in shaping stimulated reservoir volume and significantly impacting subsurface liquid production. Due to the scarcity of details on natural fractures, most research primarily focuses on regularly distributed fractures and their influence on the hydraulic fracturing process. However, these regular patterns differ significantly from actual fracture systems.

This study employs a lattice Boltzmann-discrete element method (LBM-DEM) (Galindo-Torres, 2013) to simulate the hydromechanical behavior during hydraulic fracturing (Chen & Wang, 2017, Chen et al., 2020). Additionally, we delve into the intricacies of natural fracture systems through the discrete fracture network method, incorporating these fractures into the LBM-DEM scheme. We consider two key geometrical parameters of discrete fracture networks: mean orientation and position clustering. Natural fractures are mimicked by adjusting the relative bond strength between particles. From the previous study (Zhu et al., 2023), we found that the heterogeneity of fracture strengths, injection rate, and viscosity is essential for the fracture initiation and propagation process. Therefore, in this work, we also consider different degrees of heterogeneity and injection rates under low viscosity conditions. A Taguchi design is adopted to perform orthogonal numerical tests to reduce computation time.

Preliminary observations yield several conclusions: i. Heterogeneity of bond strengths profoundly influences fracture formation and the complexity of resulting fracture systems, specifically their intensity. Extremely low bonding strength can lead to many local fractures disconnected from the primary hydraulic fracture, which, however, cannot contribute equally to production compared to the primary hydraulic fracture initiated from the perforation. ii. Higher injection rates, coupled with low viscosity, intensify fluid leakage, potentially generating extensive local fracture clusters. iii. Connectivity of hydraulic fractures increases with their propagation, positively correlating with

production rates. However, production rates are more closely tied to the total area of the primary fracture cluster. iv. In the studied cases, the geometries of fractures exhibit weak correlations with connectivity and final production rates. The clustering effect tends to enhance the connectivity of formed fracture networks and, subsequently, the final production rate.

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Poster / 171

Pore-scale Study of the Influence of Pore Heterogeneity on Non-miscible CO2 Displacing Oil

Authors: Minfeng Li[1]; Shuyang Liu[1]; Yingshuo Wan[2]; Hangyu Li[1]

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CO2 Enhanced Oil Recovery (CO2-EOR) is a green and promising technology that not only improves crude oil recovery but also reduces carbon emissions. The micro-pore structure of porous reservoirs significantly influences the effectiveness of CO2-EOR, making research in this area crucial. This study aims at the influence of pore heterogeneity on the non-miscible CO2 displacement and employs a coupled approach utilizing the N-S equations and phase-field method to numerically simulate the microscale two-phase flow of CO2-oil displacement within porous media. The impact of pore heterogeneity on the shape and stability of the CO2-oil displacement front, residual oil types, and spatial distribution are investigated under different capillary numbers. The study elucidates the mechanisms through which heterogeneity affects the non-miscible displacement process of CO2. The results indicate that, under conditions of neutral wettability ($\theta=\pi/2$) and low capillary numbers (logCa=-6.253), the increased pore heterogeneity in porous media leads to a more unstable displacement front. The overall recovery increases with an increase in capillary numbers in the model with weak heterogeneity ($\sigma=0.004$). However, the presence of dominant channels leads to a decrease in the oil recovery with the increasing capillary numbers in the models with stronger heterogeneity

(σ=0.008 and σ=0.012). With the pore heterogeneity increasing, the influence of capillary numbers on the displacement front, the quantity and spatial distribution of various residual oils, and breakthrough time become less pronounced. This research provides valuable insights into the mechanisms governing the impact of pore heterogeneity on the non-miscible displacement process of CO2-oil under different wettability and capillary number conditions for CO2-EOR.

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172

Numerical well test simulation based on fluid-thermal dual-field coupling

Authors: Qianye Xiao[1]; HONGJUN YIN[None]; Guohan Xu[None]; Qiang Lin[None]

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In the pressure unstable well testing of the reservoir with obvious temperature change, because the existence of pore fluid seepage and rock mass temperature difference is accompanied by obvious heat transfer, the seepage field and temperature field are coupled and not independent of each other. At this time, the interpretation method of isothermal well testing is obviously not accurate. In order to solve the above problems, combined with the principles of porous media percolation mechanics and heat transfer, and considering the coupling influence of reservoir thermodynamic parameters on seepage field, a fluid-thermal coupling well test model is established. Through the multi-physical field coupling simulation and well test research of the actual non-isothermal reservoir by COMSOL Multiphysics software, the typical well test curve of fluid-thermal coupling is drawn, and the curve characteristic analysis and parameter sensitivity analysis of the typical well test curve are carried out. The analysis of typical convection-thermal coupling well test curves shows that the thermodynamic parameters of core pores and reservoir fluid have a certain influence on the performance of bottom hole pressure. The research results can provide theoretical guidance for non-isothermal well testing. Keywords：heat flow coupling；energy conservation；well test；heat conductivity coefficient

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MS04 / **173**

Quantifying the Soil Swelling Potential by Soil Water Isotherm

Authors: Yijie Wang[1]; Liming HU[2]; Ning Lu[3]

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Swelling potential has long been used as a terminology to quantitatively describe the expansibility of soil. It encompasses multiple definitions such as the swelling pressure under specific strain constraints or the free swelling strain without confining stress. However, although these definitions are of great significance to engineering practice, they do not directly represent the physical nature of soil expansion. Resistance to mineral swelling occurs due to Van der Waals and Coulomb forces between crystal layers. The water adsorption ability within the interlayer space of expansive minerals can overcome this resistance by enabling water molecules to enter the interlayer space, resulting in macroscopic soil expansion. The interlayer hydration of expansive minerals serves as the intrinsic reason for soil swelling. Therefore, the authors propose utilizing the energy available for swelling of the interlayer space under a specific humidity as the soil swelling potential. To experimentally determine the proposed swelling potential, a framework based on the soil water isotherm (SWI), which establishes the constitutive relation between relative humidity and water content, was developed. SWI not only represents the energy state of soil water but also captures the interlayer water content change of expansive soil during wetting and drying through its hysteresis at low humidity. By leveraging the existing SWI model, which determines interlayer water content, and the method of calculating the water adsorption ability of soil (referred to as soil sorptive potential, SSP) using SWI, the authors can quantify the proposed soil swelling potential under any humidity. Several verifications were conducted to validate the proposed swelling potential. Firstly, the SWI of montmorillonite was generated using molecular simulation, combined with basal spacing measurements obtained from XRD tests under varying humidity. The interlayer water content and system energy change from the molecular simulation were analyzed to understand the volume change of mineral during wetting and drying. The energy change of soil-water system under humidity variations was used to verify the theoretical soundness of the established swelling potential framework. Secondly, the measured SWIs of different soil samples were utilized to calculate the swelling potential of these soils, thereby confirming the practical feasibility of the proposed framework. Finally, to facilitate comparison with existing indicators for identifying expansive soils, the energy used for crystal layer expansion during the water adsorption process, which can also be calculated using the proposed framework, was defined as the swelling potential index. This index exhibited superior performance

in identifying expansive soils compared to other indicators of soil swelling ability. This study offers a novel perspective on the study of expansive soils and establishes a scientific basis for understanding the engineering behaviors of expansive soil under varying humidity environments.

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Poster / 175

IMPACT OF DUAL POROSITY SYSTEMS ON FLOW IN HEAP LEACHING USING MICRO COMPUTED TOMOGRAPHY IMAGING

Author: Quan Zheng[1]

Co-authors: Kunning Tang [2]; Peyman Mostaghimi ; Ryan Armstrong ; Samuel Jackson [3]; Ying Da Wang [2]

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The global progress with the energy transition from fossil fuels to renewable energy has boosted the demand for metals. Copper, amongst all metal resources, is regarded as an essential raw material in producing the conduit to reduce the energy needed during electricity production. Most of the low-grade copper is recovered from heap leaching, which is a well-established hydrometallurgical method.

However, a low recovery remains a significant challenge of this method. This poor leaching performance is caused by the variation of the leaching kinetics driven by not only the leaching fluid transport at the particle scale but also the mass transport at the grain scale. Previous studies have implemented a collection of numerical and experimental methods to investigate the leaching performance under a variety of scales and leaching conditions but rarely investigated the process using a multiscale approach.

Herein, we implemented a fundametal study the flow behaviour in a dual porosity system, which is by visualising the fluid transport and measuring the liquid contents under the particle and grain scale. A series of leaching experiments is conducted using water with packed glass beads and chalcopyrite beads. We image the column in regular periods under Micro Computed Tomography (Micro-CT) imaging over several days of the leaching period. We label and track mineral grains from high-resolution images and monitor the alternation of the mineral size and porous media structure. Our study shows the impact of dual porosity systems on flow patterns and the performance of leaching on mineral grain within different particles. Our results highlight the importance of multiscale simulation for the design and optimisation of heap leaching.

Keywords: Heap leaching, dual-porosity, Micro-CT, column test

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MS06-A / 177

CT Gas Tracer Study of Gas Trapping and Diffusion in Foam in Porous Media

Author: JIAKUN GONG[1]

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Foam improves sweep efficiency in gas-injection processes to sequester CO2 in, and to produce hydrocarbons from, porous geological formations (Bellow, 2023, Rossen et al., 2022). Gas trapping plays a key role in foam's ability to reduce gas mobility in porous media. We describe a study of gas trapping and diffusion in a sandstone core using nitrogen (N2) foam and krypton (Kr) as a gas-phase tracer.

Surfactant solution and nitrogen were injected, with gas fraction 0.6, superficial velocity 2 ft/day (3.5 x 10-6 m/s), into a 17-cm-long, 4-cm-wide Berea core oriented horizontally in a CT scanner. At steady-state, foam apparent viscosity was 0.4 Pa s (400 cp), and gas saturation was uniform across the core cross-section. Then injection continued with 0.6 gas fraction, but with half the N2 replaced by Kr gas. Krypton can be distinguished in the CT scanner from N2 at the pressure of these experiments (4 MPa). Kr can therefore serve as a tracer in high-pressure foam-flow experiments in cores in place of the more-expensive xenon used by Nguyen et al. (2009). With image filters, it was possible to determine Kr fraction in the gas from the image with a resolution of about 2 mm.

CT images show that the advance of Kr was almost entirely in a thin zone at the top of the horizontal core, with trapped, immobile foam below. (See graphical abstract, where Kr is shown in red.) This is likely the result of segregation of gas and surfactant solution in the core endplate. Similar, though less-severe, segregation originating in the endplate was observed in the foam CT experiments in Kil et al. (2011). Slowly Kr diffused down from the flowing foam at the top of the core, in a similar fashion to diffusion of gas through trapped foam in the coreflood experiments in Kil et al. Our resolution was not sufficient to resolve individual flowing-gas paths in our experiments as in Kil et al., however. A model fit to the CT data indicates that flowing fraction of gas in the core was roughly 0.06, and the Kr diffusion coefficient through trapped gas was 3 to 4 x 10-8 m2/s.

In addition to measuring the flowing gas fraction and diffusion rate of gas through trapped foam, these results highlight the usefulness of Kr as a possible gas-phase tracer in high-pressure foam experiments in porous media. They also highlight the need to account for possible nonuniform injection from the core endplate in multiphase displacements in core samples.

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** Bello, A., et al., "Foam EOR as an Optimization Technique for Gas EOR: A Comprehensive Review of Laboratory and Field Implementations,"Energies, 16(2): (2023)972. https://doi.org/10.3390/en16020972 ** Kil, R. A., Nguyen, Q. P., and Rossen, W. R., "Determining Trapped Gas in Foam From CT Images," SPE Journal 16, 24-34 (2011). https://doi.org/10.2118/124157-PA ** Nguyen, Q. P., et al., "Determination of Gas Trapping With Foam Using X-Ray CT and Effluent Analysis," SPE Journal 14, 222-236 (2009). https://doi.org/10.2118/94764-PA ** Rossen, W. R., et al., "Potential and Challenges of Foam-Assisted CO2 Sequestration," SPE paper 209371, presented at the SPE Improved Oil Recovery Conference, Tulsa, OK, 25-29 April 2022. https://doi.org/10.2118/209371-MS

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Multi-scale Pore Network Modeling of a Reactive Packed Bed

Authors: Ali Fathiganjehlou[1]; E.A.J.F. (Frank) Peters[2]; J.A.M. (Hans) Kuipers[2]; K.A. (Kay) Buist[2]

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In this study, we introduce a multi-scale Pore Network Model (PNM) that uniquely integrates reactor-scale and particle-scale transport phenomena. We employ a 3D reactor-scale PNM, that is extracted from 3D structural images of a packed column with spherical particles, obtained by Magnetic Resonance Imaging (MRI). Hydrodynamic analysis of the reactor-scale PNM provides valuable insights into the flow behavior within the reactor, crucial for modeling species dispersion. Calibration of the reactor-scale PNM is performed using Particle-Resolved CFD (PR-CFD) 1 and validated by comparing the flow field from PNM to the one obtained from MRI [2]. To address particle-scale transport phenomena, we employ a 3D particle-scale PNM to simulate species diffusion and reaction within a spherical porous catalyst particle. This particle-scale PNM is reconstructed from the complex 3D pore space of a porous spherical catalyst particle, which is modeled as densely packed with numerous smaller spheres. The developed particle-scale PNM facilitates the application of realistic 3D boundary conditions on the catalyst particle's surface [3].

This work introduces an innovative methodology for coupling the reactor-scale PNM with the particle-scale PNM through the incorporation of surface fragments. The construction of these surface fragments involves applying a particle detection algorithm to structural images obtained from MRI, pinpointing the positions of spherical particles. Subsequently, each individual particle's surface is partitioned into numerous surface fragments along both azimuthal and zenithal directions. In a prior study, this specific definition of surface fragments was employed to characterize local particle wetting using MRI images of a two-phase gas-liquid flow in a trickle bed [4]. In the current research, however, this detailed partitioning facilitates the precise localization of these surface fragments within the reactor-scale volume element map, obtained from pore network extraction. So,

surface fragments of the catalyst particles can be assigned to pore bodies of the reactor scale PNM. This enables the seamless coupling of reactor-scale and particle-scale PNMs.

The multi-scale PNM developed in this study offers a computationally very efficient model, capable of swiftly generating local partially-resolved results for catalytic packed bed reactors within minutes. To validate the model, the axial concentration profile from the multi-scale PNM is compared with that from a 1D heterogeneous plug flow model for a packed bed reactor. This innovative multi-scale PNM lays the groundwork for comprehensive pore network modeling of real packed bed reactors, where a complex interplay of hydrodynamics, reactions, and mass and heat transport phenomena occurs.

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Poster / 179

Advancing Underground Hydrogen Storage: Insights from Molecular Simulations of Wettability and Interfacial Tension

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The intermittency in energy supply and demand from renewable resources, which is often caused by seasonal variations, necessitates the development of long-term energy storage solutions. One promising approach is Underground Hydrogen Storage (UHS), a scheme in which hydrogen is strategically stored in subsurface formations to maintain market equilibrium. Depleted oil and gas reservoirs and saline aquifers present an attractive option for UHS. The appeal of these reservoirs lies in their existing infrastructure and the presence of subsurface traps, which are essential for sealing

reservoir fluids. To fully leverage these reservoirs for UHS, it's crucial to understand the wettability and interfacial tension (IFT) of the gas, brine, and rock systems. These properties play a significant role in determining capillary pressure, fluid migration, and drainage in porous media. We used molecular dynamics simulations to study the impact of temperature (300 and 323 K) and pressure (5, 10, 15, and 20 MPa) on the IFT between hydrogen and formation brine. We also investigated the effects of two carrier gases, methane and carbon dioxide, on the system. Our findings revealed that the IFT of pure hydrogen/brine did not change significantly (less than 1 mN/m) with pressure. However, the addition of methane and carbon dioxide to the system lowered the IFT, with carbon dioxide having a more pronounced impact. In addition to IFT, we studied the contact angle between a gas phase (comprising hydrogen and its mixtures with methane and carbon dioxide), the brine and rock (calcite and silica) at a pressure of 20 MPa and a temperature of 300 K. With the exception of the H2-CO2/brine/silica, all systems exhibited complete water-wetting with a zero-contact angle. The exception can be attributed to the complete protonation of silanol groups, which is caused by the dissolution and hydration of CO2 to form carbonic acid, resulting in a low pH of 3. This research contributes to our understanding of UHS and provides valuable insights that could aid in the optimization of energy storage strategies. It underscores the importance of considering the effects of temperature, pressure, and carrier gases on the IFT and wettability of the system, which are critical for the efficient storage and retrieval of hydrogen in subsurface formations.

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MS11 / **180**

Conditions Allowing Steady Multiphase Flow in Microfluidic Devices

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Microfluidic devices allow direct observation of interfacial phenomena and multiphase flow in porous media. However, they have difficulty representing steady multiphase flow without fluctuating occupancy of locations in the network. The ability of two phases to form steady, intertwined flow pathways is an essential property of 3D pore networks (Sahimi, 1994; King and Masihi, 2019); fluctuating pore occupancy occurs at elevated capillary number (Gao et al., 2020). A two-dimensional network can represent this only if the flow paths of the two phases cross at some locations in the network (Fisher, 1961). Crossing is possible in a microfluidic network if wetting phase can form a bridge across the top and bottom of a gap between grains at a pore throat while nonwetting phase

flows through the throat, as illustrated in the graphical abstract, left figure.
We review conditions for existence of quasi-static flow pathways in conventional microfluidic geometries. We examine whether paths can cross in several different throat geometries (Cox et al., 2023) using the Surface Evolver software (Brakke, 1992). For relatively long straight or curved throats, the most common geometry in microfluidic networks used to study flow in geological formations (see graphical abstract, center and right figures), the capillary pressure for bridging is the same as that for snap-off. As a result, phases displace each other in turn in the network, even at the very lowest capillary number.
Concave throats, as between cylindrical barriers, can support bridges over a substantial range of capillary pressure. The range of capillary pressures at which bridging is stable increases as throats become more strongly concave (i.e., pillar radius decreases) and for narrower throats. Steady two-phase flow would be possible in networks of pores with throats of this geometry.
For networks of this geometry, we estimate the range of fractional flows of wetting and nonwetting phase that could be sustained (Obbens, 2022). To get past pore bodies occupied with nonwetting phase, wetting phase is restricted to the corners at the top and bottom of the pillars, shown in the graphical abstract, left figure. We input flow geometries determined by the Surface Evolver into the COMSOL numerical flow solver to estimate relative permeabilities of both phases for a given network realization. We choose assumptions that favor the flow of the wetting phase: for instance, penetration of the nonwetting phase just to the point where it connects across the network. The results show that the relative permeability of the wetting phase is roughly 1/10 of that of the nonwetting phase. Given the assumptions made, this is a generous estimate. If viscosities of the two phases were roughly equal, the maximum fractional flow of wetting phase would be 0.1. For gas-water studies, where the viscosity ratio can be 50:1, the maximum fractional flow of water would be 0.2%. Imposing a fractional flow above this would guarantee fluctuating pore occupancy in the network.

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Poster / 181

Testing a Thermal-Dispersion Upscaling Method for Geothermal Reservoir Simulation in Heterogeneous Reservoirs

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The lifetime of a geothermal doublet depends on the time it takes reinjected cold water to reach the hot production well. The spreading of the thermal front as it advances through the reservoir is therefore key to the lifetime of the project. Simulation of thermal dispersion in a heterogeneous reservoir is challenging. Refinement of the grid to incorporate all scales of heterogeneity is impractical. Conventional models take the arithmetic average of properties within an upscaled grid block. This causes underestimation of thermal dispersion in the flow direction.

We have developed an upscaling method that accounts for the increased "Taylor"dispersion that results from nonuniform velocities, reflecting permeability variation, within a grid block (Tang, 2022). With this method, for instance, we upscale a geothermal reservoir description with 91 layers, representing permeability values from a well log, to 12 layers (figures a and b in graphical abstract), with corrected thermal dispersion coefficients (figures c and d). The upscaled simulation model has increased thermal dispersivity in the flow direction.

In this study we examine the combined effects of improved upscaling and numerical dispersion (van Nieuwkerk, 2022) using the DARTS simulator (Khait, 2019). We use a 2D rectangular "layer-cake" model of 91 layers reflecting the permeability distribution at the well, with parallel flow to eliminate numerical dispersion from diagonal flow between grid blocks. We compare results of upscaled models to the original 91-layer description with sufficient grid resolution in the flow direction to minimize numerical dispersion overall. We examine the advance of cold water from one well to the other and, in particular, the arrival of the cold-temperature front at the production well. For simplicity, in this study we exclude heat transfer with over- and unburden to focus on dispersion within the reservoir.

With sufficient grid resolution in the flow direction, the corrected upscaling method gives a better fit to the 91-layer fine-grid model than simple arithmetic averaging within grid blocks. Upscaling in multiple stages using the new method appears to further increase thermal dispersivity by a modest amount. Arithmetic upscaling underestimates thermal dispersion.

However, coarser grid refinement (50 grid blocks between wells) increases the spread of the thermal front for both upscaling methods. As a result, combined with numerical dispersion, the arithmetic upscaling method gave a better fit in that case than the corrected upscaling. With 25 grid blocks between wells, numerical dispersion greatly distorts the results of both upscaling methods, spreading the thermal front much more than in the fine-grid 91-layer simulation.

These results show the complexity of predicting the breakthrough time of the cold-water front in a geothermal doublet. Current simulators do not account for increased dispersion arising from heterogeneity within grid blocks, but numerical dispersion greatly distorts results. Higher-order numerical methods designed to correct for numerical dispersion may help. Furthermore, if the simulator assigns the thermal conductivity automatically based on average fluid and formation properties within a grid block, it may be difficult to adjust the thermal dispersivity for Taylor dispersion.

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Impact of high concentrations of calcium ions during MICP on compressive strength, permeability and porosity of consolidated sand

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The field of geotechnology has seen growing interest in microbiologically induced calcium carbonate precipitation (MICP) as a sustainable and ecological alternative to traditional methods of mineral consolidation like cement. The most commonly used method of MICP is ureolysis, during which urea is degraded into ammonium and carbonate ions. In the presence of calcium ions and an alkaline environment the carbonate ions are precipitated as calcium carbonate. The calcium carbonate can form bri dges between particles and thereby act as binder for the particles. To achieve high compressive strengths of consolidated samples, multiple cycles of treatment with cell suspension and calcination solution (urea, calcium salts) are required. To optimize the efficiency of this process, research on the rate and kinetics of MICP has been conducted, including studies on the effects of cell concentration as well as urea and calcium concentration. However, previous research has primarily focused on low concentrations of calcium ions and cells. This study aims to gain a better understanding of MICP efficiency by investigating MICP at calcium and urea concentrations up to 2500 mM, and cell concentrations with an OD600 up to 10, which are more representative of conditions used in the production of biocement. It could be shown that the presence of calcium ions inhibits the reaction speed of ureolysis and that calcium ion concentrations above between 2000 mM and 2250 mM, depending on the cell density, lead to a complete stop of calcium carbonate precipitation. A low pH injection methodology for MICP application has gained interest in literature as an application methodology that can achieve higher homogeneity due to delaying the initial precipitation. Therefore, the influence of initial pH value on the reaction speed of ureolysis was also investigated. While at a pH value of 2 and low cell densities (OD600 1) the efficiency of MICP drops to about 60 %. At higher cell densities no impact on the efficiency of MICP could be observed, most likely due to the fast rise of pH due to ureolytic activity. It appears that for higher cell densities low pH injection of cell suspension and calcination solution this methodology is not suitable. On the basis of these findings, silica sands with different particle size distributions were treated with various injection techniques under optimal conditions based on previous experiments. The treated samples were then analyzed using micro computed tomography to determine contact points between particles and pore space volume during the MICP treatment. The results were compared with unconfined compressive strength and water permeability of the samples to find correlations between these parameters. These insights could be used to further study if reducing the duration between cycles would have any impact on the samples' compressive strength and homogeneity.

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MS06-A / 183

Trapping criteria for three-dimensional periodic liquid particles in micropillar scaffolds

Authors: Wenhai Lei[1]; Shervin Bagheri[1]; Wouter van der Wijngaart[1]

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Liquid particles within three-dimensional periodic scaffolds play a crucial role in various natural and engineering applications, for example, cellular arrays composing living tissue, 3-D materials that mimic tissue with an unprecedented level of control, and innovative liquid-infused materials designed for carbon capture. Although it has been known that fluid interfacial energy during multiphase displacement can drive the emergence of 3-D periodic liquid particles in micropillar scaffolds, the underlying microscale physics and the macroscopic formations of liquid particles in scaffolds remain unclear. Here we establish trapping criteria for the formation of liquid particles in micropillar scaffolds based on the evolution of fluid-fluid interfacial curvature during multiphase displacement, considering four key parameters (pillar size α, contact angle θ, capillary number Ca, and viscosity ratio M). The fundamental trapping criteria are theoretically derived in α-θ space under a viscous stable state and main meniscus-dominated flow, where critical α distinguishes trapping mode and complete displacement, and critical θ further distinguishes between diamond-like and spherical particles in the trapping mode. However, the critical pillar size α for trapping mode or completed displacement can be further affected by viscous instability under lower viscosity ratio M and inter-pillar interface-dominated flow under lower capillary number Ca. These criteria are validated through numerical CFD simulations and confirmed by microfluidic experiments. These results indicate the conditions for trapping 3-D periodic liquid particles in micropillar scaffolds, offering insights that extend and clarify prior literature. The derived criteria provide valuable guidelines for the design of micropillar scaffolds and for the emergence of 3-D periodic liquid particles in micropillar scaffolds under various conditions by controlling multiphase displacement processes.

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MS21 / 184

Wave-mediated diffusion model for semi-sealed systems: effective diffusion coefficient and experimental validation

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

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It is widely known that the motion of a gas at a low Mach number can be approximated as an incompressible flow at the leading order in a small Mach number expansion of the full solution (Anderson 1995; Panton 2013). However, it has been shown recently that such an incompressible approximation becomes invalid for a semi-sealed system with no inlets and no boundary movements. Studies based on linearized compressible Navier-Stokes equations for such a system made of small capillary tubes have revealed some counter intuitive flow characteristics such as no-slip flow with a slip-like mass flow rate (Chen and Shen 2018a, b; Shen and Chen 2019a, b; Shen and Chen 2020). In this work, we extend these works to a semi-sealed porous system which has applications to microfluidics and primary production from a tight gas reservoir.

Based on the compressible N-S equations and the theory of Klainerman and Majda (1982) for low Mach number flow, Jin and Chen (2019) has shown that at the pore-scale, the flow of the gas obeys a damped wave equation. Applying multi-scale analysis and volume averaging upscaling to the pore scale equation, Jin and Chen (2019) obtained a self-diffusion equation at the macroscopic scale in the limit of infinitesimal pore size. To account for small but not infinitesimally small pores, the effective macroscopic diffusion coefficient must be modified to consider the effect of wave-mediated diffusion. We first perform pore-scale numerical simulations of drainage flow from a porous plug using the damped wave equation. The mass flow rate from this simulation is then matched to the one computed from the macroscopic diffusion equation with an adjustable diffusion coefficient. The diffusion coefficient that provides such a match in the mass flow rate is then the effective diffusion coefficient.

A large number of pore scale simulations are performed for various pore structures. We study slow viscous drainage flow of a viscous compressible gas from a semi-sealed porous plug to a large vessel. The semi-sealed porous plug has a length of , height of ; and the vessel has a height of and extends to infinity downstream. We then use the homogenized medium shown in Figure 1 and the macroscopic diffusion equation with various effective diffusion coefficients to compute mass production rate from the plug. From the simulation results, it is found that the larger the porous plug length and its porosity, the larger the effective diffusion coefficient. The larger the expansion ratio, the smaller the effective diffusion coefficient. An empirical correlation of the effective diffusion coefficient is then established for applications to larger physical size. The proposed wave-mediated effective diffusion model as well as Darcy's law are both used to perform historic match with the data from laboratory experiments. The comparison shows that the wave-mediated effective diffusion model provides good agreement with experiments whilst Darcy's law severely underestimates the flow rate.

The proposed wave-mediated diffusion model is promising for applications for primary production from tight gas reservoirs. Testing of this model with field data is currently underway.

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Poster / 185

Reversing capillary trapping of nonaqueous fluid from dead-end structures by nanoparticle suspension and their self-adaptive control in complex porous media

Authors: Wenhai Lei[1]; Xukang Lu[2]; Guang Yang[2]; Shervin Bagheri[3]; Moran Wang[2]

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We report an anomalous capillary phenomenon that reverses typical capillary trapping via nanoparticle suspension and leads to a counterintuitive release of nonaqueous fluid from dead-end structures under weakly hydrophilic conditions. Fluid interfacial energy drives the trapped liquid out by hierarchical surfaces: the nanometric roughness formed by nanoparticle adsorption transfers the molecular-level adsorption film to hydrodynamic film by capillary condensation and maintains its robust connectivity, then the capillary pressure gradient in the dead-end micrometric structures drives trapped fluid motion out of the pore continuously. The developed mathematical models agree well with measured evolution dynamics of released fluid. This reversing capillary trapping phenomenon via nanoparticle suspension may be a general event in a random porous media and could dramatically increases displacement efficiency. Our findings have implications for manipulating capillary pressure gradient direction via nanoparticle suspensions to trap or release the trapped fluid from complex geometries, especially for site-specific delivery, self-cleaning, or self-recover systems.

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MS15 / **187**

CO2 Leakage Detection using Optimized Deep Learning

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1. OBJECTIVE/SCOPE
   Geologic CO2 sequestration (GCS) has been considered as a promising engineering measure to reduce global greenhouse emission. Real-time monitoring of CO2 leakage is an essential aspect of large-scale GCS deployment. This work introduces a deep-learning-based algorithm using a hybrid neural network for detecting CO2 leakage based on bottom-hole pressure measurements.
2. METHODS, PROCEDURES, PROCESS
   The hybrid neural network, called CNN-BiLSTM, leverages the strengths of convolutional neural network (CNN) and bidirectional long short-term memory (BiLSTM), in which CNN is used for spatial feature extraction and BiLSTM is applied for temporal dependency recognition. The CNN-BiLSTM enables us to build a spatial-temporal-based image-to-value regression model to learn the nonlinear mapping between high-dimensional input data (e.g., permeability, porosity, injection rate) and predicted bottom-hole pressure as output. The proposed workflow incorporates the generation of train-validation samples, the coupling process of training-validating, and the model evaluation. In this work, the diffusivity equation for pressure is solved within the CMG framework used to generate datasets under no-leakage conditions. A Bayesian optimization process is performed to optimize the network architecture, model hyperparameters, and the ratio of train to validation samples.
3. RESULTS, OBSERVATIONS, CONCLUSIONS
   We test the CNN-BiLSTM performance on the bottom-hole pressure data collected from CO2 leakage simulations. Results show that the CNN-BiLSTM model can successfully detect CO2 leakage events by comparing the difference between the predicted (no leakage) and tested bottom-hole pressures. We further compare its superiority with CNN, LSTM, BiLSTM, and CNN-LSTM. Our proposed model achieves the highest accuracy with the same datasets. The CNN-BiLSTM outperforms other models owing to 1) its capacity to process image-based input, which could accurately capture input formation, especially cases with highly heterogeneous permeability; 2) its bidirectional ability to capture time-series dependency. Other models, like LSTM and BiLSTM, take value-based input, which is insufficient to describe the input information in highly heterogeneous cases. In contrast, CNN model suffers from capturing the temporal dependency features. Because of the bidirectional feature, CNN-BiLSTM shows higher accuracy, even 10% when applied to a small number of datasets, than the CNN-LSTM model.
4. NOVEL/ADDITIVE INFORMATION
   We propose a hybrid neural network featuring Bayesian optimization for CO2 leakage detection. We demonstrate its applicability in terms of accuracy and robustness with other models. The

proposed workflow can be implemented in commercial-scale GCS for real-time monitoring applications.

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Numerical simulation of hydro-mechanical coupling in shale gas reservoirs based on coner-point grids

Authors: Jinlong Li[None]; Zhaoqin Huang[1]; Jun Yao[2]

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The flow mechanism of shale gas reservoir is complex including viscous flow, adsorption-desorption, and Kundsen diffusion, etc. The shale reservoir is usually developed by hydraulic fracturing which produces large-scale fractures. The porosity and permeability of the fractures are greatly affected by the geostress, so that the influence of the hydro-mechanical coupling effect needs to be taken into account in the numerical simulation. The reservoir geological model is usually described by corner-point grids and due to the existence of mismatched nodes in the corner-grid and complex geological structure which makes the numerical simulation of the hydro-mechanical coupling in the corner-point grids not be solved effectively. In this paper, based on coner-point grids, an effective hydro-mechanical coupling numerical simulation method for fractured shale gas reservoirs is proposed, in which the flow equations and elastic equations are discreted by the finite volume method and the virtual element method respectively, the fracture is characterized by embedded discrete fracture model and fixed-stress splitting algorithm is used to solve the flow and stress equations itetatively. The correctness of this method is verified and the effects of different parameters on gas production in fractured shale gas reservoirs are analyzed and the applicability of this method is further verified by historical fitting of actual production data.

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Shale Fracture Permeability Estimation: A Data-Driven Model Using Machine Learning

Author: Xupeng He[1]

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1. OBJECTIVE/SCOPE
   Hydraulic properties of fractures (including natural and hydraulic) in shale are essential parameters for the modeling of fluid flow in shale reservoirs. Traditional static- and flow-based methods used to estimate the shale fracture permeability suffer from low accuracy and high computation cost, respectively. Experimental measurements are even more time-consuming. This work presents a data-driven model based on machine learning as an alternative to traditional methods.
2. METHODS, PROCEDURES, PROCESS
   The objective of this study is to develop a data-driven surrogate-model for estimating shale fracture permeability, with the consideration of geometric fracture properties (e.g., mean aperture, minimum aperture, roughness, tortuosity, contact area, etc.) and other flow parameters (e.g., Reynolds number, Klinkenberg constant). The workflow for the development of the data-driven model, as shown in Figure 1, includes four main steps. Step 1: Identify uncertain parameters and perform Latin Hypercube Sampling (LHS). We first identify the uncertain parameters which affect the shale fracture permeability. We then generate ns training samples using LHS based on the identified uncertain parameters. Step 2: Perform training simulations. In this step, high-resolution simulations with parallel computing for the Navier-Stokes equations (NSEs) are run for each of the ns training samples. Step 3: Construct an optimized data-driven surrogate model. A data-driven model is then built to model the nonlinear mapping between the input and output parameters based on results collected from Step 2. Herein, four popular and powerful machine-learning techniques, including Multivariate Adaptive Regression Splines (MARS), Support Vector Regression (SVR), Random Forests (RF), and Artificial Neural Network (ANN), are implemented to select the most suitable algorithm. Step 4: Validate the proposed data-driven model. In this step, we first conduct blind validation on the proposed model with high-fidelity simulations and further test it with experimental measurements.
3. RESULTS, OBSERVATIONS, CONCLUSIONS
   We demonstrate the developed surrogate model with hundreds of fracture cases with a broad range of roughness, tortuosity, and contact area. We further extend its applicability by incorporating the inertial and gas slippage effects, which are quantified by Reynolds number and Klinkenberg constant, respectively. We then compare its performance in terms of accuracy and efficiency to the reference solutions (i.e., NSEs simulations and experimental measurements) and other seven traditional models from the literature. Results show that the developed data-driven model shows the best accuracy among the selected models. Specifically speaking, the proposed model offers

more computational efficiency than the flow-based models by two-orders of magnitude and provides more accurate results than the analytical-based models yet with the same level of efficiency. For the tested cases, the relative error of the proposed model ranges from -12 % to 10 %, with an essential normal distribution crossing the zero line and most points located within the range of -10% to 10%. Other traditional analytical- and flow-based models, however, show one-side distribution with most points either above or below the zero line, as shown in Figure 2.

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MS06-A / 190

Spontaneous imbibition in dual permeable media using dynamic pore network model

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Understanding preferential flow in porous media holds substantial theoretical significance on the design and optimization of hydrocarbon exploitation in shale reservoir. Previous researches discussed the competition of imbibition front in layered porous media while the underlining mechanism for interfacial dynamics and induced displacement efficiency of multiphase flow remains ambiguous. In this paper, we investigate the spontaneous imbibition in dual permeable media and analyze the flux exchange between the neighboring porous zones with permeability contrast using dynamic pore network model. The impact of fluid viscosity ratio and permeability contrast on the spontaneous imbibition preference have been addressed, and finally a phase diagram for displacement efficiency has been obtained. The results revealed that the dual permeable structure enhanced the invasion rate of wetting fluid in the low-permeable zone and induced unstable displacement patterns, leading to reduction of the long-term displacement efficiency. The interfacial pattern transition from stable displacement to unstable pattern in dual permeable media could be ascribed into the flux exchange between dual permeable zones, which shows a contrary impact on the fluid flow within the low-permeable zone under favorable and unfavorable viscosity ratios. The permeability contrast in dual permeable media intensifies this impact during spontaneous imbibition. These results help us to understand the occurrence and mutual interaction of multiphase flow in layered porous media, and provide a theoretical guidance for the hydrocarbon exploitation in shale reservoir.

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MS03 / 191

Study on Foam Flow Behavior in Fractured-Vuggy Systems

Authors: Zhengxiao Xu[1]; Meng Li[1]; Tong Yu[2]; Lei Tao[1]; Jiajia Bai[1]; Wenyang Shi[1]; Qingjie Zhu[1]; Zhaomin Li[3]; Zihan Gu[3]

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For deep fractured-vuggy carbonate reservoirs, foam flooding is an effective oil recovery method. However, the connectivity and anisotropy of the fractured-vuggy network affect the plugging performance of foam and the ability to adjust the displacement profile. Therefore, it is necessary to conduct a comprehensive investigation on the migration characteristics of foam, in order to provide guidance for the oilfield application of foam flooding.
The fractured-vuggy system exhibits heterogeneity and strong diversion capabilities. When developing a model that can represent reservoirs with fractured-vuggy formations, it is challenging to simultaneously satisfy the characteristics of multiple experiments with a single model. The flow behavior of foam in fractured-vuggy system is a crucial factor that needs to be observed, so it is necessary to appropriately relax the requirements for simulating reservoir temperature and pressure conditions. Based on the combination relationships of fractures, wall effects, and fluid properties, a multi-dimensional and multi-scale fractured-vuggy model was developed. This model, combined with the selected foam system, was used to study the evolution of foam structure, flow characteristics, gas-liquid distribution patterns, and oil displacement properties within the fractured-vuggy model. The study summarized the dynamic and static matching relationships between fractured-vuggy dimensions and foam, investigated the improvement effects of foam on shielding fractured-vuggy flow, and comprehensively analyzed the changes in the foam displacement front and the different distribution characteristics of gas and liquid in fractures under the influence of various factors. The study clarified the foam displacement characteristics corresponding to different production scenarios.
The experimental results show that, due to limitations in the channel dimensions, there are differences in the quantity and shape of foam distribution within fractured-vuggy formations after injection. Significant variations also exist in the evolution patterns during the static stable stage of foam. The shielding effect of foam displacement between fractures is dynamically adjusted. This is because high-quality stable foam gradually “plugs” dominant fractures, increasing the flow resistance for subsequent foam in the dominant fractures. Consequently, some foam is still able to divert towards the inferior fractures.

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MS08 / **192**

Salinity-induced melting of underlaying permafrost

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The rise of sea levels and the expansion of plateau salt lakes are among major consequences of the ongoing climate change1. When saline water overlays above permafrost (ice in porous soil), ice may melt because salinity reduces the melting/freezing point. Permafrost melting may alter the mechanical properties of the soil and affect the safety of coastal structures1, and even may induce the release of underground methane gas into the atmosphere[2]. Therefore, studying the kinetics of salinity-induced melting of underlaying permafrost is of great environmental significance.

We conducted visualized experiments to study the kinetics of permafrost melting induced by overlying saline water. Water in bead-pack is first frozen to mimic permafrost and then is immersed under excessive saline water at -5℃. Glass bead diameter varies from 0.1mm to 0.5mm, and salt concentration varies from 10wt% to 25wt%. Melting front (ice-water interface) in porous media can be visually identified (Figure 1(a)) and recorded by camera. As the dilute saline water at the melting front is of lower density than the overlying saline water, Rayleigh-Darcy convection is induced in the porous medium[3,4], so we use Rayleigh number (ratio of gravitational-induced flux over diffusion), Ra, to characterize the mass transfer in liquid-saturated porous layer[5].

Surprisingly, we found two distinct melting patterns: 1) when Ra is high, the melting front is flat and moves down stably; 2) when Ra is low, “fingers”emerge and develop at melting front. This seems to be different from the previous research results that greater Ra implies higher instability[6–8].

We theoretically show that the melting pattern is a result of interplay between local circumflux shaped by the melting front perturbation and the global Rayleigh-Darcy convection (Figure 1(b)). When a perturbation emerges at the front, density contrast induces local convection from the trough to the peak, that further enlarge the perturbation (Figure 1(c)). This local convection is proportional to Ra. Meanwhile, global Rayleigh-Darcy convection enhances lateral mixing which compress the development of the perturbation. This lateral mixing is proportional to Ra^(1.5~2). As a result, when Ra is low, melting is dominated by the local circumflux and fingers grow; when Ra is high, strong lateral mixing homogenizes concentrations along the solid-liquid interface and results in flat melting front. Numerical simulations further support the above theory and match the experiments well. When the melting front is flat, the melting rate can be predicted by classical Rayleigh-Darcy convection theory. However, when a fingering melting front forms, the melting rate is one order of magnitude slower than classical theory prediction. Moreover, fingering melting front implies penetration of permafrost layer before melting all ice, that may induce unexpected groundwater pollution and subsurface methane release.

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Poster / 195

A molecular simulation study on adsorption and diffusion behaviors of hydrogen, methane and carbon dioxide

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Because underground hydrogen storage offers the potential for large-scale, long-term storage of hydrogen, understanding the adsorption and diffusion behaviors of hydrogen and cushion gas in the reservoir is critical to understanding the underlying mechanisms that control hydrogen storage and transport. Using molecular simulation methods, we investigated the adsorption and diffusion behaviors of hydrogen, methane and carbon dioxide in kaolinite slit pores (10 MPa and 303 K), respectively. The distribution characteristics, excess adsorption amounts, diffusion coefficients and gas-solid interaction energies of the three gases in the slit pores were analyzed. Near the pore wall surface, carbon dioxide formed a distinct double adsorption layer, methane formed a smaller second adsorption layer, and hydrogen formed a single adsorption layer. The order of excess adsorption amount is carbon dioxide > methane > hydrogen. The rank of diffusivity of gases under the same conditions is hydrogen > methane > carbon dioxide. The interactions between gases and pore walls are in the following order: carbon dioxide>hydrogen>methane. Van der Waals interactions dominate. However, hydrogen and carbon dioxide have significant coulombic interactions with the pore walls, while methane has negligible coulombic interactions with the pore walls. The minerology of the formation results in different charges on the pore surfaces, which has a significant effect on

gas storage. This study provides better insights into the mechanisms of hydrogen and cushion gas storage, thus providing a theoretical basis for underground hydrogen storage site selection.

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Poster / 196

Volatile Transport in Porous Lunar Regolith: Diffusion at Infinite Knudsen Number

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The lunar surface is covered with a layer of lunar regolith. Observational evidence[1-3] suggests that it may contain volatile substances such as water, methane, and helium-3 that could be utilized. Studying the diffusion behavior of volatiles in lunar regolith is of great significance for the exploration and exploitation of these extraterrestrial resources.

Volatile in lunar regolith layer exist under extremely high vacuum conditions (~$10^{-9}Pa$)[4]. Under such extreme conditions, gas molecules undergo Knudsen diffusion, where the average free path is more than 10 orders of magnitude larger than the size of lunar regolith particles (Knudsen number $Kn > 10^{10}$). At this extreme (almost infinitely large) Knudsen number condition, gas molecules in porous lunar regolith rarely collide with each other, and the diffusion trajectories resemble chords (free paths) between solid surfaces which are determined solely by porous structure. Previous studies have measured tortuosity[5] or free path length distribution[6] to modify the diffusion coefficient, but the correlation between pore structure and the diffusion coefficient is still largely unexplored.

In this study, we investigate the influence of pore structure on the diffusion of rarefied gases in porous media at infinitely large Knudsen number, based on a Monte Carlo program. Numerical experiments confirm that the linear relationship between the mean square displacement and time predicted by the Einstein equation still holds. However, the statistics of free path lengths shows clear bimodal-distribution even in homogeneous media, which is different from the unimodal-distribution as shown in porous media Fickian diffusion or in straight tube Knudsen diffusion. By statistically analyzing the molecular trajectories within the porous medium, we show that the bimodal distribution corresponds to the sizes of pore and the throat.

According to the pore-throat bimodal distribution of free path length, we establish a bimodal random walk model to derive the diffusion coefficient from the pore and throat parameters. This analytical prediction successfully matches the numerical experiments with various structures. We further investigate the impact of adsorption and heterogeneity on the volatile transport in porous media at infinitely-high Knudsen number.

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MS17 / **197**

The evolution of water ice reservoir in lunar polar regions

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In the permanently shadowed regions of lunar polar craters, there may exist significant reserves of water ice in the porous lunar regolith (1,2), offering the potential for scalable extraction to address the water supply bottleneck for lunar bases. However, there currently are only some indirect measurements of ice content on shallow surface layer. The scale and spatial distribution of water ice underneath the lunar surface are still largely unknown.
Here we study evolution of water ice in the permanently shadowed regions at geological time scale (~billion years). We establish a three-dimensional simplified model based on the assumption of quasi-steady-state heat and mass transfer in presence of rarefied vapor crystallization and ice vaporization.

After modifying earlier approaches on dispersed fluid/cluster evolution in porous media (3), we propose diffusion and phase change equations suitable for extreme environment for ice and water vapor in lunar polar shadowed regions.
Accordingly, we are able to elucidate the dynamics of water ice accumulation & escape in polar lunar craters at geological time scale, and then estimate the scale of ice reservoirs within these specific areas. We also investigate the impact of possible sources of water ice within permanently shadowed regions: a) ice crystals brought by incoming meteorite impacts, and b) water vapor migration from low-latitude regions to high-latitude regions on the lunar surface (4, 5). We further provide projections for the distribution of water ice over a billion-year timescale, which may help the selection of water recovery sites in future lunar missions.

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Poster / 198

Relative permeability curve prediction directly from 3D digital rocks based on AI approaches

Authors: Jingwei Zhu[None]; Hongqing Song[1]; Chiyu Xie[None]

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The relative permeability curve is one of the key features to evaluate the flow property of a porous medium, which is important in many subsurface engineering problems such as underground energy storage and recovery. Recently, rapid developments in the technology of artificial intelligence (AI) have offered new views to revisit the acquisition of relative permeabilities. Here, we present our systematic work on the developments of AI models for the predictions of relative permeability curves directly from 3D digital rock images. The training and testing data are generated from pore-network simulations and core-flood experiments. It avoids the use of indirect geometrical parameters as inputs in previous AI methods. It is able to cover 3D digital rocks with variable sizes

and further equiped to have the upscaling capability. The results show that the AI models have high prediction accuracies over 95%, with scale information being the most important physics feature accounting for 51%, and the upscaling prediction of relative permeability curve is in good agreement with macroscopic experiment data. The new framework is also flexible and can be easily extended for the prediction of other rock physical properties according to practical demands.

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MS06-A / 200

Microfluidic experimental study of CO2-water-oil three-phase flow in porous media

Author: Shuxuan Zhang[1]

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Understanding the mechanisms of CO2-water-oil three-phase low is crucial for enhancing oil recovery and improving CO2 storage efficiency. In the present study, with the help of high pressure high temperature microfluid experimental system, the pore-scale CO2-water-oil three-phase flow is directly visualized and the underlying mechanisms of triple-phase flow are revealed.
During the experiments, the contact angle of the microfluidic porous chip is altered to study the triple phase flow with different wettability In water-wet systems, water tends to occupy the small pores, oil exists in the intermediate pores, while CO2 enters the large pores. Gas ganglia disconnected with continuous gas injection do not reconnect and CO2 is displaced in the form of disconnected ganglia by a double/multiple displacement process. In contrast in the oil-wet system, , a three-phase Haynes jump occurs in the pore space during oil replacement by gas.
Under supercritical conditions, it can be observed that the oil droplets are extracted during gas displacement. The CO2 displacement in oil-water filled porous chip which has been already displaced by water can further reduce the oil saturation. The residual oil presents in the form of columns, membranes and corners. In addition, as the gas injection rate is increased from 0.005ml/min to 0.01ml/min, the residual oil content is reduced from 42.11% to 18.35%, indicating greatly enhanced oil recovery. When the gas injection rate is further increased to 0.02ml/min, the increase of the oil recovery is negligible, due to the occurrence of gas channeling.

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MS03 / **201**

Countercurrent imbibition in shale with parallel dense fractures: analytical model and anisotropic relative permeability

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Countercurrent imbibition is the process that the wetting phase spontaneously displace the nonwetting phase in porous media while the nonwetting phase is recovered at the wetting phase inlet1. It is a major mechanism of shale oil recovery, where the permeability is so low that co-current imbibition is largely limited[2, 3]. For fractured media, classic dual-porosity model is based on good fracture connectivity and assumes that fractures are evenly distributed into each grid[4, 5]. Although the heterogeneity and anisotropy of porous media are considered in some dual-porosity models, they mainly assume topologically connected fracture network [6, 7].

However, in continental shale reservoir, the distribution and morphology of fractures are very unique. As shown in Fig. 1a , continental shale consists of very densely-packed parallel microfractures. On one fold, fractures are not directly connected, that breaks the assumption of continuous fracture phase in dual-porosity models; on the other fold, the distance between neighboring microfractures are extremely small (100-500 micrometers)[8], so they are hydrodynamically highly correlated by coupling and not independent. Unfortunately, there is still no suitable REV (representative elementary volume) scale model to describe imbibition in such parallel dense fracture system.

In this study, we first numerically simulate the countercurrent imbibition in a dual- unidirectional microfracture system using MRST with fine grids, using typical continental shale parameters. Two distinct stages are identified: an early stage that fractures can be treated as independent, and a late stage that neighboring fractures are strongly correlated by capillarity. In both stages cumulative oil production grows proportional to the t^0.5(shown in Fig. 1), while with different pre-factors. We show that the late stage is the dominant stage in shale oil recovery. After elucidating the mechanisms of fracture-fracture capillary interaction, we successfully derive analytical solution for countercurrent imbibition kinetics at the late stage, and accordingly propose equivalent REV models for both systems. The REV model is validated with fine-grid simulation.

Notably, we find that anisotropic relative permeability is required to depict imbibition in such parallel dense microfracture system at REV scale. This is distinctive from classic approaches for modeling anisotropic media where simply adopting anisotropic absolute permeability is adequate. It brings new challenge in numerical simulation at reservoir scale.

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Core-Scale Modelling of Cyclic Creep Deformation During Cyclic CO2 Injection and Storage in Unconventional Reservoirs

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Cyclic CO2 injection, followed by soaking, and production [”Huff-n-Puff” (HNP)], can be employed in unconventional reservoirs to reduce greenhouse gas emissions while increasing oil recovery. Cycles of unloading and loading stress occur during HNP due to gas injection and gas-oil production,

which in turn lead to cyclic strain accumulation and subsequent creep deformation. This study investigates the impact of cyclic creep deformation on CO2 storage and enhanced oil recovery (EOR) using experimental data and numerical simulation with a focus on the matrix and fracture flow.
Intact and naturally fractured core plugs from the Canadian Montney Formation (tight siltstones) were tested in this study. Single-phase gas flow (gas permeability) measurements were carried out under multiple cycles of loading and unloading stresses, followed by the determination of slip-corrected permeability, porosity, compressibility, effective diffusion coefficient, and Biot's coefficients for each cycle. The measured data were utilised to develop hydromechanical models to study the physics of cyclic CO2 injection and storage in fractures and pores of the rock at the core scale. Various deformation scenarios were considered, encompassing conditions where the rock was rigid, elastic, weakly elastic, and subjected to cyclic creep (plastic). The geomechanical behaviour was assessed with coupled multiphase, multicomponent flow and transport models. Furthermore, a series of sensitivity simulations were conducted to study the influence of different confining stresses on the HNP flow characteristics.
The results indicate that cyclic creep deformation affects CO2-EOR processes as rock and flow properties, such as permeability and porosity, diminish with each successive cycle, with a more pronounced effect on fractures than matrix. As the number of cycles increases, the accumulated creep deformation leads to a slower pressure build-up during CO2 injection and a slower depletion rate during oil production. Consequently, CO2 storage is reduced by 18% and 30%, and oil recovery by 5% and 20% in pore and fracture domains, respectively, compared to models without creep effects incorporated. The results also demonstrate that free and dissolved CO2 storage volumes increase with each cycle. However, fractures allow for significantly greater dissolved CO2 storage, 21%, compared to only 6% in matrix-only models. Additionally, a noticeable progressive reduction in diffusive CO2 flow across cycles highlights a gradual shift from diffusion-dominated to convection-dominated flow due to reservoir depletion. With increasing confining stress, effective stress also rises, which leads to reduced porosity but enhanced free CO2 storage, particularly in the initial cycles, with a more pronounced effect on the fracture than the matrix system.
Ignoring the effect of cyclic creep deformation can overestimate oil recovery and CO2 storage capacity. This highlights the need for accurate modeling with creep effects incorporated in order to optimise the number and duration of cycles in CO2-EOR schemes. Although the potential for cyclic CO2 storage in the analysed Montney interval is limited, the prospect for dissolved CO2 storage in these reservoirs appears promising. Creep-informed models help to enhance our understanding of subsurface responses in cyclic CO2-EOR and storage schemes, which provides some insight into the development of sustainable energy systems and efficient carbon management strategies.

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MS15 / 205

Deep learning-assisted technology transition in natural hydrogen development

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Although the global energy sector is shifting from the fossil-based energy systems to the renewable energy resources, the conventional energy development techniques has received increasing attentions with the mature development and the recharge by AI. With the help of AI techniques, drawing lessons from thousands of years of traditional energy development in the technology transition into the next-generation energy is an effective approach to accelerate energy transition and avoid repeated research causing unnecessary wasting. In this talk, we will introduce an iterative flash calculation scheme and a deep learning algorithm using a thermodynamics-informed neural network (TINN) to perform accurate, robust, and fast phase equilibrium calculations for realistic fluid mixtures of natural hydrogen. The development of natural hydrogen is an emerging topic in the current energy transition trend. The production process involves compositional multiphase flow via subsurface porous media. This makes studying the compositional phase equilibrium behavior essential for reliable reservoir simulation and prediction. The application of TINN architecture can accelerate the calculations for nearly 20 times. The effect of capillarity on phase equilibrium states is demonstrated. Based on simulation results, suggestions for the natural hydrogen industry chain are provided to control the possible phase transitions under certain environmental conditions that may be observed in the natural hydrogen reservoirs, storage and transportation facilities. The extremely low critical temperature of hydrogen challenges the robustness of flash calculations but facilitates the separation of impurities by liquefying certain undesired species. Moreover, phase transitions under control can be an effective approach for carbon dioxide capture and sequestration with optimized operating conditions over the phase equilibrium analysis.

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Poster / 206

Analysis of CO2 huff and puff displacement effect of shale oil in Block A

Author: sen deng[1]

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In response to the low porosity and permeability of shale oil reservoirs in Block A, as well as the difficulty in producing shale oil, nuclear magnetic resonance experimental technology and high-temperature and high-pressure CO2 huff and puff experimental technology were used to study the

effects of shale oil huff and puff pressure, extraction rate, maturity, and shale oil composition on CO2 huff and puff oil recovery efficiency, and to explore the occurrence characteristics of shale pore fluids in the T1-T2 two-dimensional spectrum. The experimental results show that the rapid extraction of shale oil is 7.43 percentage points higher than the slow extraction, but excessive pressure drop in the formation can cause strong stress sensitivity, and the actual production process needs to optimize the extraction speed; The extraction rate of high maturity shale is 11.13 percentage points higher than that of low maturity shale. Optimizing favorable desserts for development is an effective method for energy conservation and efficiency improvement; When the throughput pressure approaches the formation fracture pressure, it can significantly increase the shale oil recovery rate; After CO2 huff and puff, shale oil still retains immovable oil in large pores and bedding fractures in the T1-T2 two-dimensional spectrum.

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MS03 / **207**

Non-Local Flow Description for Non-Space-Stationary Fractured Formations

Author: Shangyi Cao[1]

Co-authors: Daniel Stalder ; Daniel Meyer [2]; Patrick Jenny

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Flow in fractured porous media plays an important role in applications ranging from geothermal energy production to the selection of suitable underground CO_2 storage sites. Predictions of flow and transport are central in these applications and often times corresponding models are applied that rely on effective permeabilities. In subsurface formations, where fractures extend over distances comparable to the scale of interest, such models are no longer suitable. As an alternative, a model based on conductivity kernels has recently been proposed. This model accounts for the non-local character of long-range flow conduits or fractures leading to a description, which is based on an integro-differential equation. In this work, this model is extended for non-space stationary fracture statistics with model predictions being successfully compared against fracture-resolving reference simulations.

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MS03 / **209**

A New Numerical Well-Test Model Using an Analytically Modified Embedded Discrete Fracture Model

Author: Zhiming Chen[1]

Co-author: Wei Yu [2]

[1] *China University of Petroleum at Beijing*

[2] *The University of Texas at Austin*

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The technology of multi-stage, multi-well pad fracturing is an effective way to increase the stimulated volume and recoverable reserves in shale reservoirs. During the fracturing treatments, there are common phenomena of well interferences from the multi-well pad. However, there still lacks an effective tool to analyze the parent-child interactions and to evaluate the fracture parameters quantificationally. To narrow this gap, a numerical pad-well model is developed for pressure transient analysis in fractured horizontal wells with secondary fractures and well interferences, based on a discrete fracture model (DFM) and unstructured PEBI grid system.

Using methods of automatic differentiation and Newton iteration, the proposed model is more efficient for computations and interpretations of well testing curves. Its accuracy and practicality have been demonstrated by model verifications and field applications. The results show that the flow regime of interference effects caused by parent-child interactions are more obvious, with a larger child-well production, a smaller well spacing, and a larger hydraulic-fracture angle. The well interferences are also stronger when the child well has more secondary fractures, longer secondary fractures, and higher fracture conductivity, as the pressure drop caused by child well will propagate more quickly. Once the complex fracture networks have developed within the multi-well pad, the interactions between parent and child well will be weaker with the increase in area and conductivity of fracture networks. By comparison, the pressure transient behaviors of Parent well are remarkably affected by Child-well production rate, well spacing as well as connectivity degree. However, the angle, length, number, and conductivity of secondary fracture have weaker impacts on the pressure transient behaviors of Parent well. The field application shows that the single-well testing model without considering well interference cannot match with field data at the late stage. In this case, the estimation errors will occur. With considering the well interferences, the well testing data are interpreted and the fracture parameters are evaluated successfully. This work provides a meaningful way to understand the pressure transient behaviors and to evaluate the fracture parameters of multi-stage, multi-well pads.

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Baca, R. G., Arnett, R. C., and Langford, D. W. 2010. Modelling fluid flow in fractured-porous rock masses by finite-element techniques. International Journal for Numerical Methods in Fluids 4 (4): 337-348. https://doi.org/10.1002/fld.1650040404. Chen, Z., Liao, X., Zhao, P. et al. 2021. A Well-Testing Approach for Diagnostics of Fracture Complexity with Well Interference. Proc., SPE Annual Technical Conference and Exhibition. https://doi.org/10.2118/206197-MS. Deruyck, B. G., Bourdet, D. P., DaPrat, G. et al. 1982. Interpretation of Interference Tests in Reservoirs With Double Porosity BehaviorTheory and Field Examples. Proc., SPE Annual Technical Conference and Exhibition. https://doi.org/10.2118/11025-MS. He, Y., Cheng, S., Qin, J. et al. 2018. Analytical interference testing analysis of multi-segment horizontal well. Journal of Petroleum Science and Engineering 171: 919-927. https://doi.org/10.1016/j.petrol.2018.08.019. Huang, Z., Yan, X., and Yao, J. 2014. A Two-Phase Flow Simulation of Discrete-Fractured Media using Mimetic Finite Difference Method. Communications in Computational Physics 16 (3): 799-816. https://doi.org/10.4208/cicp.050413.170314a.

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MS13 / **211**

Calculation of CO2-oil minimum miscibility pressure for tight reservoirs considering adsorption effect

Author: Zengding Wang[1]

Co-authors: Keli Ding [2]; Jun Yao [2]; Tengyu Liu [2]; Hai Sun [2]; Yongfei Yang [2]; Lei Zhang [2]; Mojdeh Delshad [3]; Kamy Sepehrnoori [3]; Junjie Zhong [2]

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CO2 miscible injection holds tremendous potential for enhancing tight oil recovery, where achieving the minimum miscibility pressure (MMP) is crucial. The adsorption of CO2 and oil in nanopores affects the CO2-oil MMP in tight reservoirs, necessitating the precise calculations of nanoscale MMP and a comprehensive understanding of influencing factors. In this work, we employed a modified Peng-Robinson equation of state (PR-EOS) for nanoscale MMP calculations, incorporating adsorption layers and effective molar volume to describe molecular adsorption. Additionally, our improved method accounted for capillarity and critical point shift. The accuracy of this approach is validated against molecular simulations and nanofluidic experiments, with a maximum deviation of 4.61%. We observed that in nanopores, achieving miscibility demands less CO2 than in bulk. The CO2-oil MMP reduces as pore size decreasing, influenced by adsorption, capillarity and critical point shift. At 5 nm, the MMP is 11.12 MPa, 27.8% lower than the bulk value (15.4 MPa). Adsorption intensifies this reduction by curtailing free molecules and effective pore radius, and becomes more pronounced for lighter hydrocarbon mixtures. However, the nanoscale CO2-oil MMP is equal to the bulk value when rp ≥ 350 nm. Furthermore, a maximum MMP and the corresponding transition temperature exist for each pore size, and increase as pore size increasing. This method provides a valuable tool for optimizing CO2 miscible injection and carbon storage in challenging nanoscale-pore reservoirs.

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Poster / 212

A study on the CO2 displacement behavior at nanoscale considering rough surface

Author: Keli Ding[1]

Co-authors: Hai Sun [1]; Jun Yao [1]; Junjie Zhong [1]; Yongfei Yang [1]; Zengding Wang [1]

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CO2 displacement is considered as a potential method to enhance shale oil recovery. CO2 can reduce the viscosity and surface tension of crude oil, making it possible to recover crude oil in the nanopores. At the same time, the CO2 can also be partially stored underground, reducing the carbon footprint of the hydrocarbon extraction process. Therefore, understanding the CO2 displacement in nanometer pores of shale is critical for developing effective CO2 injection techniques. In this work, we applied direct numerical simulation to study the effect of rough surface on CO2 displacement in nanometer pores of shale. By quantifying the CO2 displacement in rough nanochannels, we aim to understand how surface roughness and morphology affect the displacement process. After considering the influence of slip effect, the CO2 displacement process in three channel models was studied (single channel, pore throat structure, nanoporous media). We found that in a single channel, the rough surface leads to the reduction of CO2 displacement paths, slowing down the displacement rate. In addition, the pinch-point effect of the rough nanochannel prevents the smooth progression of the interface contact line. The Periodic fluctuations at the interface further hinder CO2 displacement. The smoother the convex and convex transition of rough surface, the smaller the resistance effect of the pinch-point effect. In the pore throat structure model, the rough surface makes it easier for residual oil to remain in the pore. We also simulated CO2 displacement in rough nanoporous media and found that rough surfaces lead to a substantial reduction in CO2 displacement efficiency. Our simulation results show that the surface roughness of shale nanometer pore has nonnegligible effect on CO2 displacement.

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Poster / 213

Experimental study on microscopic pore-scales crude oil production characteristics and influencing factors during dynamic imbibition of shale reservoir with online NMR

Authors: Meng Du[1]; Shuyi Lu[None]; Zhengming Yang[1]; Lanlan Yao[1]; Weifeng Lv[2]; Pengwei Fang[1]; Qainhua Xiao[None]

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Dynamic imbibition and displacement between the matrix and fractures in shale reservoirs can significantly enhance oil recovery (EOR) following initial depletion. However, the microscopic production characteristics and seepage mechanisms at different pore scales during the dynamic imbibition process remain incompletely understood. In this study, we established an online physical simulation experiment method that combines dynamic displacement and imbibition based on nuclear magnetic resonance (NMR), and a series of online NMR water flooding dynamic imbibition experiments were conducted. Through real-time dynamic monitoring of multiphase flow and migration behavior of crude oil in each stage of dynamic imbibition, the microscopic production characteristics and influencing factors were quantitatively studied from the recovery and residual oil saturation field distribution of different scale pores, the contribution mechanism of imbibition and displacement to EOR were investigated, and the multiphase and multi-scale dynamic imbibition crude oil migration and seepage models are discussed. The results show that shale oil occurrence pores can be categorized into two types based on the corresponding production mode (imbibition + displacement). The imbibition effect predominantly governs the recovery of small and large pore walls, while displacement primarily occurs in large pores and fractures. The water flooding dynamic imbibition process in shale reservoirs unfolds in three stages: strong displacement and weak imbibition stage characterized by the rapid production of large pores and fractures under displacement action; weak displacement and strong imbibition stage involving the slow production of small pores under reverse imbibition; and dynamic equilibrium stage characterized by weak displacement and weak imbibition. Viewing the entire water flooding dynamic imbibition process as an organism, it becomes imperative to maximize the recovery of large pores while ensuring the recovery degree of small pores. High permeability contributes to better pore throat connectivity, shorter imbibition equilibrium time, and a greater imbibition and displacement production degree. The contribution of the two production modes to the recovery of small and large pores increased by 4.67% and 3.17%, respectively. A negative correlation was observed between high displacement pressure and imbibition recovery, yet it is conducive to the contribution of displacement to total recovery. Notably, fractures can effectively increase the imbibition contact area, reduce oil-water seepage resistance, and increase the contribution of displacement to recovery by 21.65%. Effectively utilizing the bridge flow conductivity of fractures is crucial for improving matrix oil production. This study provides theoretical support for clarifying the interaction between matrix-fracture imbibition and displacement and for the efficient development of shale oil.

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MS15 / **214**

A Comprehensive Approach to In-Situ Stress Estimation in Subsurface Energy Structures using Numerical Simulation and Machine Learning

Authors: Aboozar Garavand[1]; Fahimeh Hadavimoghaddam[2]; Erfan Mohammadian[None]

Co-authors: Masoud Mostajeran Gortani [3]; WEI Jianguang [4]; Xiaofeng Zhou [5]

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The objective of this research is to establish a consistent relationship between nonlinear numerical simulations and the obtained results for use in inverse analysis. We simulate the shape of breakouts, taking into account inelastic deformation of high-porosity limestone, using developed finite element methods under various in-situ conditions. Subsequently, the dataset is employed to train four machine learning algorithms, as well as white-box algorithms, in order to determine the relationship between in-situ stress and breakout shape.

This study employs a two-phase approach through inverse analysis to determine in-situ stress. In the initial phase, we utilize nonlinear elastoplastic finite element modeling to generate a dataset. This dataset serves as the training data for a machine learning (ML) algorithm designed to establish a predictive correlation between in-situ stress and borehole breakout measurements. In the second phase, the trained ML algorithm is applied to estimate the equivalent in-situ stress based on provided borehole breakout measurements. To investigate in-situ stress from borehole breakouts and construct robust correlations, we employ a combination of four black-box algorithms and three white-box algorithms.

A numerical simulation has been performed to determine the geometry of borehole breakouts under various in situ stress levels and taking into account plastic deformations. The breakout cross-section's non-circular shape can be modeled using an elastoplastic model that was created using the finite element approach. This shape fluctuates as the breakout develops until it stabilizes. The depth of the breakouts rises until a stable state, just like in earlier models based on the elastic assumptions.

The width of the breakouts, however, does not change as the breakouts develop. The growth of the breakout is stopped by taking into account inelastic deformations, which also gives the chance to model the V-shaped type breakouts seen in both field and laboratory data. According to laboratory research, disregarding plastic deformations in very porous and weak rocks results in an incorrect understanding of the relationship between in situ stress and rock failure state.
To determine the correlation between in situ stress and breakout shape, four machine learning techniques and three whitebox algorithms have been applied to the data set generated from numerical tests. To calculate the in situ stress from breakout shapes, trained algorithms were put through an inverse analysis. The XGBoost and GP algorithms mean square error (RMSE) of 0.419541, 0.9977and a determination coefficient (R2) of 0.99565 and 0.97564 outperform others in terms of accuracy and suitability.
The novelty of the proposed approach lies in its consideration of inelastic deformation for estimating in-situ stresses, which is a crucial factor in the failure of high-porosity and unconsolidated rocks. Additionally, it involves establishing a relationship for estimating in-situ stresses through a combination of machine learning and numerical simulation.

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Physics-embedded inverse analysis with algorithmic differentiation for the earth's subsurface

Author: Hao Wu[1]

Co-authors: Daniel O'Malley [1]; Sarah Greer [2]

[1] *Los Alamos National Laboratory*

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Inverse analysis has been utilized to understand unknown underground geological properties by matching the observational data with simulators. To overcome the underconstrained nature of inverse problems and achieve good performance, an approach is presented with embedded physics and a technique known as algorithmic differentiation. We use a physics-embedded generative model, which takes statistically simple parameters as input and outputs subsurface properties (e.g., permeability or P-wave velocity), that embeds physical knowledge of the subsurface properties into inverse analysis and improves its performance. We tested the application of this approach on four geologic problems: two heterogeneous hydraulic conductivity fields, a. hydraulic fracture network, and a seismic inversion for P-wave velocity. This physics-embedded inverse analysis approach consistently characterizes these geological problems accurately. Furthermore, the excellent performance in matching the observational data demonstrates the reliability of the proposed method. Moreover,

the application of algorithmic differentiation makes this an easy and fast approach to inverse analysis when dealing with complicated geological structures.

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MS11 / 217

A Novel Microfluidic Approach to Quantify Pore-Scale Mineral Dissolution in Porous Media

Author: Rafid Musabbir Rahman[1]

Co-authors: Colin Shaw [1]; Yaofa Li [1]

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Mineral dissolution in porous media coupled with single- or multi-phase flows is pervasive in natural and engineering systems. In subsurface environments, the solid porous matrix is composed of various types of minerals, through which subsurface water flows. Dissolution of minerals occurs as chemicals in the solid phase are transformed into ions in the aqueous phase, effectively modifying the physical, hydrological, and geochemical properties of the solid matrix as well as the chemistry in the aqueous phase. These processes play a defining role in a broad range of applications such as carbon capture and sequestration (CCS), underground contaminant transport and vadose zone sciences. For instance, CCS is considered as a viable technology to reduce carbon emissions to the atmosphere, thus effectively mitigating global climate change. However, injection of CO2 into geologic formations leads to dissolution of minerals, potentially comprising reservoirs rocks, and creating leakage pathways that threaten the safety and security of CO2 storage. Therefore, to successfully model, predict, control, and optimize these many processes, a comprehensive understanding of mineral dissolution is crucial.

Mineral dissolution in porous media and pore flow are strongly coupled. On the one hand, pore flow plays a defining role in mixing and transporting the reactants to the reaction sites as well as transporting reaction products away. On the other hand, mineral dissolution modifies the porous media both structurally and chemically, in turn reshaping the pore flow. However, our fundamental understanding of this coupling effect at the pore level is still limited, leading to strong challenges in the effort of predicting mineral dissolution at much larger scales. To this end, mineral dissolution is studied in novel calcite-based porous micromodels under single- and multiphase conditions, with a focus on the interactions of mineral dissolution with pore flow. The microfluidic devices used in the experiments were fabricated in calcite using photolithography and wet etching. These surrogate porous media offer precise control over the structures and chemical properties and facilitate unobstructed and unaberrated optical access to the pore flow with μPIV methods.

The preliminary results provide a unique view of the flow dynamics during mineral dissolution. It is observed that the local dissolution rate is strongly affected by the local pore flow, with much higher dissolution rate in fast flow regions and lower dissolution rate in slow flow regions. This process significantly reshapes the geometry of individual calcite grain, in turn posing feedback to the flow. Additionally, when HCl concentration is sufficiently high, the produced CO2 emerges as a separate phase, leading to a multiphase flow. The separate CO2 phase not only divert the HCl flow, but also shield the solid surfaces from further reaction, thus significantly modifying the local dissolution pattern and rate.

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MS06-B / 218

Contact angle on rough curved surfaces and its implications in porous media

Authors: Lei Liu[1]; Liang Lei[1]

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Equilibrium contact angle depends on both the chemistry of the two fluids and solid base, and the microstructure on the solid surface. Actual surface of the pore wall in porous media is typically rough and curved, which has not been well-considered in related applications. This work uses a free interfacial energy minimization approach to theoretically derive the equilibrium contact angle on two specific surface structures on flat surfaces and extends the derivation considering the surface curvatures in porous media. Results reveal the equilibrium contact angle is not dependent on the curvature of spherical surfaces, and we further prove that this conclusion applies to any point along the apparent common line at solid surfaces with any arbitrary curvature. The fundamental physics is the local mechanical balance of a composite contact among three interfacial tensions. Furthermore, the contacting mode can shift from non-wetting to wetting when the pressure difference between two fluids exceeds the entry pressure of the microstructures, which should be considered in relative dynamic scenarios such as rain droplet impact and fluid displacement in porous media. Note these conclusions are from pure theoretical analysis based on idealistic assumptions and real circumstance may deviate from these assumptions.

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Poster / 219

Mechanism and Control Factors of Particle Migration in Loose Sandstone Reservoirs

Authors: Bowei Liu[1]; Chunsheng Jia[2]; Hongming Tang[3]; Yawei Hou[1]; haoxuan tang[2]; zhao wang[4]

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Particle migration and plugging are ubiquitous throughout the entire lifecycle of unconsolidated sandstone reservoir development. During the extraction process, particle migration and plugging alter the microscopic characteristics of the reservoir, while the microscopic parameters of the reservoir control particle transport and plugging. This paper utilizes methods such as CFD-DEM, visualization of laser-etched pore structure models, dynamic core displacement, and thin-section casting to systematically discuss the coupled relationship between the microscopic characteristics of unconsolidated sandstone reservoirs and particle migration. This includes the impact of particle size, concentration, particle/pore throat ratio, pressure drop. Based on particle transport/plugging in different types of pore structure models. The achievements and understanding are as follows: Based on particle size, reservoir particles are categorized into seepage sand (<4μm), formation particles (4~32μm), and framework particles (>32μm). When particle volume concentration is >1%, particles are more likely to be retained on the pore surface and in the throat. When the particle size/throat is less than 1/14, the migration of permeable sand has almost no effect on the permeability of the reservoir. When the particle size/throat is less than 1/7, particles will aggregate and settle in the pores. When the particle size/throat is less than 1/7, particles will disperse and settle in the pores. When the particle size/throat is greater than 1/3, particles will bridge and block the throat in the form of single double particles or multiple particles. This study proposed that the migration/blockage of particles in reservoirs has periodicity, stages, and persistence. This paper evaluated the differences in particle migration and blockage in different types of reservoirs, and established a coupling relationship between the permeability damage rate of particle migration and the microscopic characteristic parameters of the reservoir. And established three mechanisms and six modes of particle and blockage in loose sandstone.

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Poster / 220

Prediction model of permeability in porous media with different arrangements

Authors: Yang Zhang[1]; Bei Wei[1]; Jian Hou[1]

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Corresponding Authors: b23020041@s.upc.edu.cn, sllx_upc@126.com, bwei@upc.edu.cn

Abstract:
Permeability is a measure of flow resistance in porous media. As an important characterization parameter of porous media flow capacity, it is widely used in oil/gas development, filtration analysis, groundwater transport, hydrocarbon recovery and so on. However, on the one hand, the permeability was considered a monodrome function of porosity by many researchers in their studies [1~3]. On the other hand, its determination for different types of porous media is challenging due to its complex dependence on the pore-scale structure of porous media [4], which always includes fractures caused by hydraulic fracturing and geological factors.
We first established an absolute permeability computational method to determine the actual relation between permeability and other pore-throat parameters. The method is based on the Darcy equation and Lattice Boltzmann method (LBM). Then we calculated the permeability for porous media with different pore-throat parameters. A modification to the Kozeny-Carman equation was made by considering the effects of pore-throat ratio and coordination number. Finally, we studied the impact of fracture and arrangement. The compound porous media (CPM) with different initial porous media (IPM) structures and arrangements, such as series connection and parallel connection, were constructed and the compound permeabilities were calculated. According to the electric resistance network analogy [5], the relationship between the compound permeability and the permeabilities of IPM was established mathematically.
Using the LBM, our revised permeability calculation method matched well with the theoretical prediction compared to the classical Kozeny-Carman equation. In low-permeability tight reservoirs or shale reservoirs, fracture contributes more to fluid transport rather than matrix, which was confirmed by its higher permeability. Besides, our calculation results revealed that the arrangement, while directly affecting the compound permeability, will further affect the compound permeability by changing the tortuosity. This effect through tortuosity is more pronounced in CPM with series connection.

Key words: *Permeability, Lattice Boltzmann method, Kozeny-Carman equation, Porous media arrangement*

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MS13 / **222**

Investigation of Fluid Flow Mechanism Considering Multi-Component Fluids, Nanopore Roughness, and Nanopore Flexibility

Authors: Tianhao Li[1]; Hai Sun[1]; Zheng Li[2]; Dongyan Fan[1]; Lei Zhang[1]; Jun Yao[1]

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Understanding the occurrence and flow mechanisms of shale oil in nanopores, as well as the impact mechanisms of fluids on solid deformation, is crucial for advancing our comprehension of fluid behavior in porous media. Prior neglect of factors such as the multi-component characteristics of shale oil, the properties of real shale nanopore walls, and nanopore flexibility has resulted in insufficient knowledge regarding the occurrence and flow mechanisms of shale oil in nanopores. In this study, molecular dynamics simulations were employed to extensively investigate the occurrence and flow mechanisms of fluids in graphene, hydroxylated quartz, rough kerogen rigid nanoslits, and flexible nanotubes. The following conclusions were drawn: (1) The occurrence patterns of multicomponent shale oil in organic and inorganic nanopores were revealed. The adsorption characteristics of shale oil are related to the pore wall elements. Components containing oxygen, nitrogen, and aromatic hydrocarbons tend to adsorb more readily on quartz surfaces, while sulfur-containing components also tend to adsorb on the kerogen surface due to interactions with sulfur elements in kerogen. (2) Real shale oil flows in real nanopores without slippage. Through simulations comparing the flow of single/multicomponent shale oil in smooth/rough nanopores, we found that slip phenomena occur only under ideal conditions (single-component oil, smooth surface). The slip does not occur in realistic shale oil flow, offering theoretical support for setting slip length in pore-scale simulations. (3) In quartz, kerogen, and graphene nanoslits, an increase in pore pressure was observed with the elevation of pressure gradients. In rigid graphene nanoslit, fluid flow induces an elevation in nanoslit pressure, with a critical pressure gradient of 1 MPa/nm. Below this threshold, pore pressure exhibits minimal variation; above it, a significant increase is observed. Higher pressure gradients lead to an increase in kinetic energy in the direction perpendicular to the wall, indicating an escalation in collision intensity between the fluid and the wall, as well as among fluid particles, resulting in a rise in pore pressure. Increased pressure gradients reduce the interaction energy between the fluid

and the wall, signifying that fluid molecules are propelled further from the wall upon collision, underscoring the gradual intensification of fluid-wall collisions. (4) The intricate relationship between pressure gradient, nanopore stress, and nanopore strain was revealed. Under static conditions, the transition of a rigid and smooth nanopore to a flexible one can result in an increase in surface roughness, which leads to a reduction in the density of the adsorption layer. The pore width decreases and the pore pressure increased slightly. Fluid flow induces an increase in pore pressure and width. Simulations of fluid flow in rigid nanoslits with coupled pore width and rock compressibility, as well as in flexible nanotubes, indicate that an increase in pressure gradient leads to pore expansion. This study revealed the intricate interactions of shale oil in nanopores, offering theoretical support for understanding its flow in porous media and contributing to the efficient extraction of shale oil from unconventional reservoirs.

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Poster / 224

Study on the pore-scale multiphase seepage characteristics of clayey-silt sediments

Author: Yuxuan Xia[1]

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The sediment of natural gas hydrate reservoir in the South China Sea is primarily composed of clayey silt, exhibiting characteristics such as loose structure, lack of consolidation, high clay content, and complex pore structure. These features contribute to the complexity of reservoir seepage characteristics, making it challenging for conventional experimental methods to accurately describe the evolution of permeability and the main controlling factors. By combining seepage experiments with micro-CT, the seepage characteristics and distribution patterns of multiphase fluids at the pore scale are obtained. The results indicate that in single-phase water seepage experiments, the pore structure of clayey-silt samples undergoes creep as the seepage process progresses. With increasing seepage pressure, the pore and throat radius of the samples decreases, leading to a significant decrease in permeability. In gas displacement experiments, fluid in larger pores is initially displaced, and with increasing displacement pressure, water in smaller pores is further displaced. The gas phase permeability gradually increases, and when the displacement pressure exceeds the initial consolidation pressure, the sample generates the dominant flow channels composed of fractures. Once the dominant flow channels appear, the gas phase permeability remains constant. The two-phase relative permeability curves of the samples are obtained through gas-water displacement experiments, showing a narrow range of co-permeability for both phases, lower co-permeability point, and high bound

water saturation. The research findings help clarify the multiphase seepage characteristics during the development of clayey-silt natural gas hydrate, providing theoretical guidance for improving recovery efficiency of hydrate reservoirs.

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MS04 / **225**

Role of Substrate Roughness in Soil Desiccation Cracking

Authors: Yuhan Yang[1]; Chao Zhang[1]; Lingyun Gou[1]; Renpeng Cheng[1]; Yi Dong[2]

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Soil desiccation crack is ubiquitous in nature, yet the physics of its initiation and propagation remain under debate, as it involves complex interactions across multiple fields of mechanics, hydraulics, and thermals. Here, an experimental attempt is made to uncover the role of substrate roughness on the soil desiccation process. The substrate roughness is deliberately fabricated by 3D printing, whereas the thickness of sample and environmental humidity are controlled to eliminate the effect of large hydraulic gradient. Four types of soils with varying expansibilities were desiccated on substrates with varying roughness. It reveals that: (1) soil desiccation crack evolution can be conceived as a competing process between the shear failure of soil-substrate interface, i.e., slippage of interface, and the tensile failure of soil, i.e., crack initiation, in minimizing the total energy of drying soil; (2) substrate roughness alters the failure mode and shear strength of soil-substrate interface and its sensitivity to moisture, thereby it regulates the pattern of how soil crack propagates upon drying; (3) soil expansibility is recognized as a key factor governing the crack-initiation point in addition to the widely recognized air-entry, and flaws in soil are the sources for the 120° crack angle and bimodal crack angle distribution.

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MS10 / **226**

SEM image segmentation based on deep learning

Author: Ziyun Zhang[1]

Co-author: Chuanzhi Cui [1]

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Image segmentation techniques for processing scanning electron microscopy (SEM) images can enhance the efficiency of oil and gas field exploration. This study initiates by reviewing the limitations of traditional SEM image segmentation methods (threshold-based, boundary-based and region-based), especially the challenges in processing complex structures and high-noise images. Subsequently, the basic principle of deep learning technology in image segmentation is deeply discussed, with a specific emphasis on the superiority of Convolutional Neural Network (CNN) architectures such as Fully Convolutional Networks (FCN) and U-Net in SEM image segmentation research. Finally, the challenges facing the current research are analyzed, encompassing difficulties in data annotation, the enhancement of model generalization capabilities and the processing of multi-modal SEM images. Prospects for future research directions are also put forward.

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MS15 / **227**

Solving seepage equation using physics-informed residual network without labeled data

Authors: Shuaijun Lv[1]; Daolun Li[1]; Wenshu Zha[1]; Luhang Shen[1]; Yan Xing[1]

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Physics-informed neural network (PINN) is an innovative universal function approximator which adds physical constraints to neural network to make the fitting results satisfy the physical laws better. In this paper, a physics-informed residual network (PIResNet) is proposed to solve the single-phase seepage equation without labeled data. The loss function is constructed by summarizing the residuals of the discretized seepage equation based on the finite volume method (FVM), and the boundary conditions are embedded in the PDE residuals in a "hard constraint"way. The PIResNet is simple in network structure, fast in convergence and easy to optimize. Furthermore, the convergence of the residual structure used in this paper is proved and the theoretical analysis of time complexity illustrates the computational efficiency of PIResNet. The correctness of the proposed method is proved and the experiments display that the solution time of PIResNet is reduced by more than six times compared to physics-informed convolutional neural networks (PICNN). (Note: This paper has been published in Computer Methods in Applied Mechanics and Engineering.)

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MS13 / 230

Slip correction theory and transient solution of the pressure oscillation method

Author: Mingbao Zhang[1]

Co-authors: Moran Wang [1]; Zhiguo Tian [1]

[1] *Tsinghua University*

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The pressure oscillation method is a widely employed technique for measuring the permeability of time-varying and tight porous media. The previous analytical solution for permeability calculation neglects the unsteady-state condition of the slip effect, and the application of the Klinkenberg correction lacks theoretical support. Existing permeability calculations rely on the periodic part, and the utilization of the transient part needs further development. In addition, parameter regulation in experiments incurs trial-and-error costs, and the reasonable prediction of parameter setting is necessary. In this study, the analytical solution of the pressure oscillation process considering the slip boundary is derived based on the capillary model and perturbation expansion. The correspondence between the Klinkenberg correction relation and the Knudsen number is clarified, which provides a theoretical basis for applying Klinkenberg correction to the pressure oscillation method. A new data processing method is proposed for permeability calculation based on the transient solution, and the scope of application of the Klinkenberg correction for the new method is given. Experiments of

the pressure oscillation method and pulse decay method are carried out to validate the theoretical model and data processing method. Through comparison of the permeability measurement results, the transient solution is consistent with the periodic solution, and the unification of the quasi-steady-state and unsteady-state methods under pressure oscillation conditions is achieved. In contrast to the pulse decay method, the pressure oscillation technique exhibits advantages in terms of measurement duration. Under conditions of higher permeability, a tenfold increase in measurement speed can be attained, while under lower permeability conditions, there is a minimum threefold improvement. Through the inverse solution process for permeability calculation, this study analyzed the main factors influencing measurements in the pressure oscillation method. The reason for the inaccuracy of porosity measurement is that porosity is extremely sensitive to the amplitude ratio and the phase difference, and the measurement error is magnified several times. The contour of the amplitude ratio response based on the dimensionless number is established to provide a reference for the selection of experimental parameters for practical engineering applications.

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Poster / 232

Theoretical Foundation for Klinkenberg-corrected Permeability of Microporous Media in Pulse Decay Method

Author: Tian Zhiguo[None]

Co-author: Moran Wang [1]

[1] *Tsinghua University*

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We provide the theoretical foundation of directly adopting the Klinkenberg plot, the apparent permeabilities versus the reciprocal of the mean pressures, in Pulse Decay Method to eliminate the slippage effect, which is characterized by the Knudsen number and strengthens with the decrease of permeability, by asymptotic perturbation of Navier-Stokes equation in capillaric model in this work. Traditional late-time solution of Pulse Decay Method intrinsically cannot take the slippage effect into account, except for some tedious numerical attempts. We theoretically fill the gap of interpreting the experimental data got by the traditional late-time solution of Pulse Decay Method with consideration of the slippage effect. By considering the nature of the low value of permeability, asymptotic perturbation method is adopted to theoretically solve the governing equation. We show that the Klinkenberg plot can be safely used to interpret the experimental data of Pulse Decay Method for microporous media when the ratio between the pore volume of the microporous media and the upstream or downstream chamber is smaller than 0.1. This implies that when one chamber, upstream or downstream chamber, is totally sealed in experiment, the slippage effect cannot be eliminated for this kind of experimental apparatus. Our own experimental results, by comparing

the intrinsic permeabilities got by Pulse Decay Method and steady-state method in different mean pressures for the same sample, verify the correctness of our derivation.

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MS11 / 233

Self-organized colloidal streamers in porous media: Emergence, development and clogging consequence

Authors: Xukang Lu[1]; Han Xiao[2]; Junlin Luo[1]; Wenbo Gong[None]; Moran Wang[1]

[1] *Tsinghua University*

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Colloidal particles from industrial and natural sources can alter the environment they flow through. Colloidal retention and accumulation in porous media may cause catastrophic consequences, such as fouling of filtration membranes, formation damage in geological systems and thrombosis in human bodies. It can also be utilized in many aspects, including enhanced hydrocarbon recovery and targeted drug delivery. Therefore, prediction of retention and accumulation mode is crucial for understanding colloidal transport in porous media.

Conventional description of colloidal transport in porous media is based on filtration theory and core-scale measurements, where the collector efficiency serves as a comprehensive parameter reflecting all particle interactions with the medium. Recent advances in microfluidics have provided tremendous insight into pore-scale particle behaviors. Geometrical confinement in porous media is the most common origin of clogging, such as size exclusion and bridging effects. Physicochemical interactions also drive particle accumulation by promoting surface deposition and aggregation under favorable conditions. Previous studies mainly focus on the direct interaction between intercepted particles and surrounding medium, leading to increased flow resistance at narrow throats. However, the self-organization of colloids under constrained porous flow condition is overlooked.

In this work, we report unexpected formation of colloidal streamers in porous media. Microfluidic experiments with high-speed imaging system combining bright field and fluorescence observations enable us to visualize the emergence and development of self-organized particle structures. Streamer formation is initiated by particle retention in the stagnant zone between solid grains, where the interparticle adhesion contributes to the connection and thickening of streamer structures. Colloidal streamers are found to be ubiquitous by constructing regular arrays with various packing arrangements and densities. Balance between fluid shear force and particle-wall adhesion determines the

extension state of these streamers, which is confirmed under oscillate boundary conditions. Numerical simulation with developed model based on computational fluid dynamics and discrete element method reproduces our experimental observations. The triggering mechanism and criterion for streamers are further clarified via theoretical analysis. When introduced into disordered porous medium, streamer development is further strengthened due to the complex geometry. Clogging consequences are observed and quantified for upscaling of streamer impact. Our results reveal the existence and importance of self-organized colloidal streamers, deepening understanding of microscopic colloidal behaviors with macroscopic flow consequences during transport in porous media.

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MS03 / 234

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

Author: Renjun Zhang[1]

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

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Suspended particle migration and clogging processes in rock fractures are ubiquitous in nature and industrial activities like hydraulic fracturing and hole-drilling fluid leakage resistance. As a common type of particle cohesion, the impact of liquid cohesion on clogging in rock fractures and its mechanism remain unclear. We conduct visualized experiments and discover that even if a small amount of immiscible liquid phase is added into the particle suspension, the clogging in fractures is significantly enhanced. By varying the flowrate and secondary liquid content, four patterns of particle clogging behaviors are found. The reason for clogging enhancement is further explained by the particle agglomeration induced by capillary cohesion. To quantify the effect of capillary cohesion, we propose a theoretical model of agglomerate size distribution as a function of various secondary liquid content and a criterion for particle agglomerate clogging in rock fracture. These findings have potential applications in numerous field applications involving particle migration and clogging, including oil/gas exploitation, drilling fluid leakage resistance, and drilling cuttings underground disposal, etc.

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Zhang, R., Yang, Z., Detwiler, R., Li, D., Ma, G., Hu, R., & Chen, Y. F. (2023). Liquid cohesion induced particle agglomeration enhances clogging in rock fractures. Geophysical Research Letters, 50(5), e2022GL102097.

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Poster / 235

Stages of change in the permeability of the chalk core during the injection of produced water and seawater

Author: Maksim Kurbasov[1]

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Chalk reservoirs, because of their high porosity and very low permeability, represent one of the most interesting cases for carbonate engineering studies. They exhibit complex fluid-rock interactions due to their reactive surfaces and tight porous environment. Re-injection of co-produced water is an attractive strategy for managing the wastewater stream from oil wells, however, the reactive nature of carbonates and the permeability presents challenges with permeability loss. Identifying the stages and understanding the processes that occur during the reinjection of produced water into a well is necessary for planning correct technological operations to increase the permeability of the formation and the feasibility of these operations. This study examines the stages of permeability change during the re-injection of produced water and seawater from the Danish North Sea oil and gas fields. Using computed tomography, real core samples from the chalk formations were selected to be homogeneous without any open fractures. All experiments were carried out in a core flooding system simulating well conditions with respect to pressure and temperature. Produced water samples were taken from the Dan field to replicate the chemical and thermodynamic processes occurring in a real well as accurately as possible. As a result of the core flooding experiments, 3 stages of core permeability changes were identified (permeability increase, pressure stabilization, and permeability decrease). The processes occurring at each stage of the change in permeability were explained based on the data of the chemical composition of produced water from an ion chromatography-mass spectrometry, image analysis from a scanning electron microscope, measurement of particles size by a zetameter, as well as building a thermodynamic model of scale formation in ScaleCERE software. These experiments provide new data for the process of changing the permeability of oil fields consisting of chalk reservoirs and additional evidence for existing theories.

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Afekare, D. A.; Radonjic, M. "From Mineral Surfaces and Coreflood Experiments to Reservoir Implementations: Comprehensive Review of Low-Salinity Water Flooding (LSWF)". Energy Fuels 2017, 31, 13043−13062, DOI: 10.1021/acs.energyfuels.7b02730 Akhmetgareev, Vadim , and Rais Khisamov. "40 Years of Low-Salinity Waterflooding in Pervomaiskoye Field, Russia: Incremental Oil." Paper presented at the SPE European Formation Damage Conference and Exhibition, Budapest, Hungary, June 2015. doi: https://doi.org/10.2118/174182-MS Beath J.M and Boone M.A. (2012) Real-world Environmental impact assessment of hydraulic fracturing. Proceeding of The Air and Waste Management Association' s Annular conference and Exhibition, 3, 1960-1965 Bergfors, S. N. (2020). Produced water chemistry - Analysis of produced water from the Danish North Sea: Inorganic ions, heavy metals and organic compounds. Technical University of Denmark Borazjani, Sara , Chequer, Larrisa , Russell, Thomas , and Pavel Bedrikovetsky. "Injectivity Decli

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Poster / 236

Remobilization mechanism of microscopic residual oil in heterogeneous sandstones during water flooding process

Author: Qi Zhang[None]

Co-author: Yongfei Yang [1]

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The displacement of residual oil by water flooding in porous media is important in many sandstone reservoirs. Our fundamental understanding of the influence of complex pore geometries of natural sandstones on fluid distribution is still incomplete. To study the formation mechanism and mobilization potential of microscopic discontinuous residual oil, this paper constructs a two-phase flow simulation model in heterogeneous sandstone pores based on the N-S equation and fluid volume method (VOF). The pore structure characteristics are accurately described using the watershed method, and the relationship between residual oil distribution and pore structure parameters was quantitatively characterized. Our findings suggest that pore-scale displacement and snap-off processes have a strong dependence with the coordination number, pore radius and aspect ratio. Moreover, the micro remobilization mechanism of different types of residual oil is analyzed from a hydrodynamics perspective. The results show that the residual oil of network form is the main type during the high-water period influenced by the low coordination number of heterogeneous pore space. Mechanical analysis shows that the mobilization of residual oil is the result of the combination of capillary force and driving force during low-capillary number water flooding process. Pores with good connectivity are the potential breakthrough positions for oil phase. The increasement of driving force would further push the two phase interface to move and form a combined force with the capillary force, and effectively remobilizing oil clusters. The statistical analysis revealed that the development of subpathways and the suppression of snap-off are responsible for the decrease of remaining oil saturation under higher capillary number water injections. This study reveals the formation and remobilization mechanism of microscopic residual oil in the high-water cut stages, providing a theoretical basis for fine tapping of the highly disconnected remaining oil in sandstone reservoir.

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MS10 / **237**

Experimental study on optimization of acidizing acidizing fluid in heterogeneous oolitic limestone reservoir

Author: Yanying Qu[None]

Co-author: Dongjin Xu [1]

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The oolitic limestone reservoir of Qianjiang Formation in Jianghan Oilfield has the characteristics of shallow burial, thin layer, developed upper and lower water layers and strong heterogeneity, so it is difficult to be reformed on site. In order to optimize the transformation process and the optimal process parameters suitable for the reservoir, the core dissolution experiment and acid displacement experiment of two different acid systems of conventional acid and retarded acid were carried out in this paper. Combined with the analysis of CT scanning results, the action law of oolitic limestone and different acid systems, the quantitative characterization of permeability change at different injection rates and the CT three-dimensional imaging of acid etching pore characteristics were clarified; at the same time, according to the results of acid rock reaction kinetics experiment and acid etching conductivity experiment, the effective distance of acid rock reaction in different acid system is predicted theoretically, and the best acid system and injection parameters are optimized. The results showed that the optimum concentrations of hydrochloric acid and retarded acid were 20 % and 10 %, respectively. The displacement rate has no obvious difference in the increase of permeability after core acidification, but it has a great influence on the wormhole structure formed by acid etching. The increase of displacement rate will form wormholes with better connectivity and less damage to rock skeleton and physical properties; by calculating the experimental parameters of acid-rock reaction kinetics, it is found that the effective distance of retarded acid is 10 m longer than that of conventional acid under the same injection rate of large displacement acid. Finally, according to the characteristics of the reservoir, a large displacement injection of ‘ 10 % retarded acid + 0.3 % corrosion inhibitor ‘ acid system can effectively increase the acid action distance and enhance the transformation effect.

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Poster / 238

Upscaled model for steady slip flow fluid structure coupling in shale system

Authors: Yurou Sun[1]; Hai Sun[2]; Xia Yan[2]; Dongyan Fan[2]; Lei Zhang[3]; Shuaishi Fu[2]; Jun Yao[2]

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Shale is a highly heterogeneous porous material rich in organic matter. Injecting fluid into a porous material can expand the pore space, distorting the solid skeleton. The detailed flow and mechanics of this solid deformation has not yet been systematically investigated. This work reports on modelling steady liquid flow in shale system, considering the slip effect and fluid-structure wall deformation. A microscale (pore level) fluid structure interaction (FSI) problem is formulated in terms of incompressible Newtonian fluid and a linearized elastic solid. The slip effect is adopted means of a Navier-type boundary condition. Combining different mechanical properties of organic and inorganic matter, an asymptotic solution to the FSI problem is derived for a certain geometry. A nonlinear Darcy-type upscaled equation for the averaged pressure is obtained, as well as introducing an apparent permeability dependent on interface position and slip coefficient. Based on the obtained results, relevant results for more general situations are obtained through extended analysis. The accuracy of the result is assessed by comparisons with numerical simulations. Our results may be useful for a better understanding of shale oil rocks at the micrometer scale, studying the large squeezing deformation of carbonaceous shale in practical situation or studying the deformation of other porous media.

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MS09 / 239

Role of micro-fractures on displacement of immiscible fluids in fractured porous media: a pore-scale perspective

Authors: Zhennan He[1]; Yinglong Zhang[1]; Pei Zhao[1]; Yan Zhou[2]; Ning Qin[1]

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Displacement of immiscible fluids in heterogeneous porous media is extensively found in many underground applications, such as groundwater remediation, underground hydrogen storage (UHS), and geological carbon storage (GCS). Natural fractures are widely distributed in the subsurface system and likely to induce a channeling effect that makes the flow within fractured porous media very distinct from that in conventional ones. In pursuit of enhanced displacement efficiencies in the aforementioned applications, the mechanisms of flow phenomena within fractured porous media needs to be better known by accounting of the channeling effect. Here, based on a numerical phase-field method (PFM), the spatial and temporal evolution of the phases and their interface during a multiphase flow in a fractured porous media are investigated under various fracture morphologies (i.e., aperture, length, dip angle, and tortuosity). The results show that the absolute permeability of the porous medium is all increased in the studied cases due to the presence of microfractures. This increase in permeability is largely attributed to the reduced fluid tortuosity in the flow direction. Yet the ultimate displacement efficiency shows a non-linear dependence on the absolute permeability. Micro-fractures serve as a main displacement pathway in view of the varying topology of the local pores, and thus play a key role in controlling the ultimate displacement efficiency. Among the above four characteristic parameters, aperture has the most significance in regulating the fluid displacement. The ultimate displacement efficiency reaches a maximum value (51.14%) as the aperture of the micro-fracture is twice the mean pore diameter and can be 1.2 times larger than that of the model without micro-fractures. The relative permeability of the displacing fluid, which is proportional to its saturation, shows a higher growth rate under presence of micro-fractures. It is also demonstrated that the ultimate displacement efficiency is negatively correlated to the growth rate of relative permeability.

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Streamline-Enhanced Dynamic Grid Sampling for Addressing Data Sparsity in Well-Based Surrogate Reservoir Modeling

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With the growing expansion of machine learning applications in reservoir proxy modeling, the effective design of input and output data for data-driven models remains a formidable challenge. This challenge is particularly pronounced due to the diverse nature of available data, encompassing variations in type, quantity, and accessibility. As the demand for robust reservoir models intensifies, overcoming these hurdles becomes imperative for harnessing the full potential of data-driven approaches. In response to this critical need, our study addresses the pivotal challenge of utilizing reservoir grid data efficiently for model training associated with well-based Surrogate Reservoir Modeling (SRM), highlighting the significance of the grid sampling method as a key solution to enhance model efficiency and accuracy amidst inherent well's data sparsity concerns. Conventional approaches treating each grid's data as a distinct observation become impractical, diminishing the efficiency of network training with an extensive array of input variables. Real-world reservoirs, often comprising tens of thousands to several million grids, intensify this complexity, emphasizing the necessity for a practical approach to reflecting the reservoir's evolving behavior over time into a designed Spatio-Temporal database for data-driven model training.

To overcome these challenges, we present the Streamline-Enhanced Dynamic Grid Sampling technique, a novel methodology integrating streamline simulation data into grid sampling. The core tenet is to capture reservoir grid data dynamically, considering fluid flow progression within the reservoir. Unlike static or random sampling approaches, our method adapts dynamically to evolving reservoir conditions, ensuring a more accurate representation of the reservoir's behavior during the training phase of the surrogate model. The methodology comprises two pivotal components: a database reflecting the inherent nature of reservoir fluid flow and a versatile application seamlessly integrating across diverse reservoir geometries. This approach conquers the limitations of existing methods, providing the physics of flow in the database structure.

To illustrate the effectiveness of the introduced method, a deep learning-based SRM is designed and applied based on the introduced data sampling technique for a water flooding process in the Egg reservoir model. The significance of this benchmark lies in its representation of real-world complexities and its acceptance within the reservoir simulation scope. The method's superiority over conventional static and random grid data sampling is assessed by the surrogate model's ability to mitigate data sparsity issues. The results demonstrate that with the introduced method, the developed SRM requires a lower database for convergence while enhancing the simulation accuracy of well production rates compared to conventional well-based surrogate models.

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MS11 / 241

Robust determination of viscosity of surfactant-polymer solution for enhanced oil recovery using microfluidics approach

Author: Wenbin Gao[1]

Co-authors: Debin Kong [2]; Qi Li [1]; Yiping Wen [1]; Yiqiang Li [3]

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Objective:
It is believed that viscous oil-displacement fluids enhance oil recovery (EOR) by modulating the mobility ratio between displacement fluid and oil. According to classical mobility control theory, a lower viscosity ratio of the defending fluid and the invading fluid would allow for better incremental oil recovery. However, core-scale experiments have shown that the viscosity ratio is not always monotonically related to incremental oil recovery. Instead, there is an optimal viscosity. The determination of viscosity for non-Newtonian fluids, which are the primary composition of chemical flooding, is inherently elusive. This has become an important issue in the application of chemical oil-displacement agents to reservoirs. While core-scale experiments can aid in viscosity design, extensive experimental work can impede research progress. Microfluidic is an advanced technique that enables in-situ visualization within porous media. In this study, we propose a microfluidic approach to enable rapid decision-making on the viscosity of viscous chemical oil-displacement agents.
Method:
Microfluidic experiments using PDMS chips were conducted to perform surfactant-polymer (SP) experiments at different polymer molecular weights and concentrations. The experimental results were analyzed using our previously proposed image algorithm (Gao,2021) for multi-scale pore recovery coupling with z-score method, which allows for characterization of the viscosity matching degree in different planar pore radii. Finally, the hydraulic radius approach is applied to upscale the planar pore radius in microfluidics to permeability of the reservoir. This enables the graphical plotting of matching degree between reservoir permeability and apparent viscosity.
Results：
The microfluidic experimental results confirm that higher viscosity does not lead to better incremental recovery. Instead, there exists an optimal viscosity. The viscosity of the displacement agent and the pore have a matching relationship, and a higher matching degree corresponds to a higher recovery. For HPAM-based SP solutions, a lower viscosity is observed at lower pore radii. With average pore radius in the range of 3-14μm, the most appropriate viscosity is in the range of 9-42cP. In same viscosity SP solutions, a high concentration of low molecular weight was found to be more effective in EOR than a low concentration of high molecular weight. The reason for this is that higher concentration gradients are conducive to the mobilization of residual oil in the smaller pore spaces.
Novel：
This work provides new insights into the microfluidic applications for EOR. Compared to extensive core experiments, microfluidics offers the advantage of characterizing mobilization in multi-scale pores simultaneously. This approach requires only a few experiment to achieve the same results as more than a dozen core-scale experiments, thus significantly reducing the effort and time required. On the other hand, microfluidics has the advantage of allowing in-situ visualization in porous media, which facilitates the understanding of the performance and mechanism of chemical oil-displacement agent, and has the potential to replace core-scale experiment to some extent in phenomenological research.

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Poster / 242

Do capillary and film water have equal matric suction or not in simple geometries ?

Author: Zi Li[1]

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The pore water retained in the unsaturated soil includes film water stagnant on the solid surface and capillary water in corners or pores, which can be morphologically quantified by film thickness and radius of meniscus curvature, respectively. The current procedure and theory of soil water retention (SWR) measurement assume that capillary water and film water are connected in the medium saturation range and have equal suction values when they coexist especially in the clayey and loamy soils. However, the results of theoretical derivation and numerical simulations from this work reveal that the film thickness remains constant with the varying radius of meniscus curvature, not following the classical relationship. Moreover, the adsorptive suction is much higher than the capillary suction and the adsorptive interaction on solid boundary affects the shape of SWR curve significantly. These findings not only help to establish the SWR function with accurate physical meanings in the field of soil physics and hydrology, but also have important implications for understanding the general relationship between film thickness and meniscus curvature as well as measuring the disjoining pressure isotherm in colloid chemistry and interface science.

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Poster / 244

Microfluidic study on the gas-water flow behaviors at pore-scale in tight sandstone rocks

Author: Jian Tian[1]

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Gas-water two phases flow behavior is fundamental to understand the underground gas exploitation. Due to the limitations that core-scale displacement experiments cannot reveal the evolution of gas-water interface and distribution of gas and water at pore-scale, a visualization study of gas-water two-phase flow at pore-scale using microfluidics was conducted in this study. Both a single capillary model and pore network model were designed based on CT images of real tight sandstone rocks and related microchip models were fabricated and etched. Then the dynamic evolution of gas-water interface and flow phenomena at pore-scale were investigated using these two micro models. The core-scale flow experiments were also carried out to analyze the gas and water flow mechanisms. The results shows that snap-off and bypass flow were the two most important pore-scale events that occurred during the evolution of gas-water interface to break the continuity of gas flow. Once the gas phase is discontinuous, the Jamin effect became remarkable to hinder the gas flow and water drainage, resulting in gas entrapment and residual water produced. Combined with the core-scale analysis and pore-scale visualization, the damage mechanisms of water blocking in tight sandstone reservoirs is elucidated from the perspective of pore-scale evolution of gas-water interface. These findings will improve the knowledge of gas-water flow mechanisms and reveal the intrinsic mechanism of the water blocking in tight formations.

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MS03 / 245

Generalized framework for flow in fractured subsurface formations

Author: Daniel Stalder[None]

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While isolated fractures are difficult to fully characterize in subsurface formations, they serve as highly conductive long-range flow conduits and thus may have a strong influence on flow and transport. Recently, we have proposed a new model for flow in fractured formations that provides predictions of the expected flow field. Unlike existing methods, this model accounts for the non-local effect of these flow conduits using kernel functions that appear in an integro-differential flow balance equation. In the present work, kernel functions predicting mean flow rates and pressure profiles for a variety of fracture shapes are presented. Furthermore, discrete fracture length distributions are incorporated leading to a formalism that can account for mixtures of different fracture families. A series of numerical experiments are presented with the results being successfully compared to expensive fine-scale reference simulations.

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MS09 / 246

Regularization strategies to improve the numerical efficiency of a fully-implicit pore-network model

Author: Hanchuan WU[None]

Co-authors: Martin Schneider [1]; Maziar Veyskarami ; Rainer Helmig [1]

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Porous media coupled with free-flow systems are prevalent in both natural and technical applications. A classic example of such systems in the nature is the interaction between wind and partly saturated soil, leading to soil drying through evaporation. In fuel cells, as an example of technical applications, the understanding of interface process between the free flow (gas distributor channel) and the porous medium (gas diffusion layer) is crucial for optimizing fuel cell performance. In order to simulate these strongly non-linear coupled systems, efficient, monolithic model concepts are required.

Pore-network model (PNM) has been proven to be an efficient tool to capture pore-scale phenomena. Through simplified representation of porous media geometry, a pore-network model describes the porous medium as large void spaces, pore bodies, connected by narrow paths, pore throats. In this work, we focus on the fully implicit pore-network model and discuss the related modeling and numerical challenges. A central concern in this type of pore-network models is dealing with the discontinuity in local conductivity of fluid phases due to displacement processes, i.e., invasion and snap-off, in the pore throat, which causes numerical convergence issues during simulation. To tackle this issue, we first propose regularization strategies to smoothen the local conductivity curve. In addition, we introduce a generalized flux function formulation using a Heaviside function to scale the flux within a pore-throat with a factor parameter. We analyze the impact of employing the aforementioned approaches on the numerical efficiency and accuracy of the fully-implicit pore-network model. Finally, we show that the further development of our PNM allows simulating porous media coupled with free-flow systems.

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MS23 / 247

Spontaneous fragmentation of dissolving ganglia in porous media

Author: Kangdi Xu[1]

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After injecting CO_2 into subsurface porous media for sequestration, CO_2 may be trapped as continuous gas cap (structural trapping) 1 or dispersed ganglia (capillary trapping) [2]. The former can utilize local pore space more efficiently, while the latter has been well-recognized to be hydrodynamically more stable. After thousands of years, both gas cap and gas ganglia dissolves into formation fluid. However, the evolution of ganglia and gas cap during slow dissolution in porous media is still largely unexplored.

We conduct experiments on slow dissolution of gas in porous media into surrounding liquid. Surprisingly, the ganglia dissolution is not in classic "outside-in"mode that the ganglia interface flinches inward gradually, but in a counterintuitive "inside-out"mode: liquid bridges spontaneously emerge at the throats after several hours and finally fragment the ganglia into pieces. One example in the micromodel visualized experiment is shown in Fig. 1a. Intriguingly, it suggests a probability that structural trapping can spontaneously transform into capillary trapping during mild dissolution, which helps to achieve stable CO_2 storage without sacrificing space utilization at the very beginning.

We hypothesize that this counterintuitive phenomenon, which emerges when large ganglia slowly dissolve, is driven by the optimization of free energy, i.e., forming liquid bridges is a thermodynamically more optimum pathway than outside-in dissolution. To prove this hypothesis, we first employ a conceptual 2-D theoretical model [3] to analyze thermodynamic states of ganglia in homogeneous porous media. We confirm that in porous media with narrow throats, dissolving bubble by forming liquid bridge is of lower free energy than by outer boundary flinch [Fig 1.b]. Kinetically, the liquid bridge can form via 1) film flow when liquid is completely wetting, and 2) capillary condensation of connate water via Ouzo effects when the liquid is only partially-wetting.

We further develop quasi-static pore network modeling (PNM) algorithm to extend the experimental discovery and theoretical interpretation into 3D and heterogeneous media. Pore bodies and pore throats are depicted as spheres and cylindrical tubes for simplicity. This PNM successfully identifies the thermodynamically optimum pathway of ganglia dissolution, and quantifies the quasi-steady state mass transfer coefficient between two phases [Fig 1.c]. We show that "inside-out dissolution" path results in larger mass transfer coefficient than "outside-in"path [Fig 1.d], which may facilitate dissolution and mineral trapping in subsequent stages.

In summary, we reveal a novel mechanism in CO_2 subsurface sequestration that continuous gas and large ganglia may spontaneously break into pieces via forming liquid bridges during dissolution. This "inside-out"pathway is thermodynamically more favored. It provides a new perspective to estimate sequestration efficiency and safety.

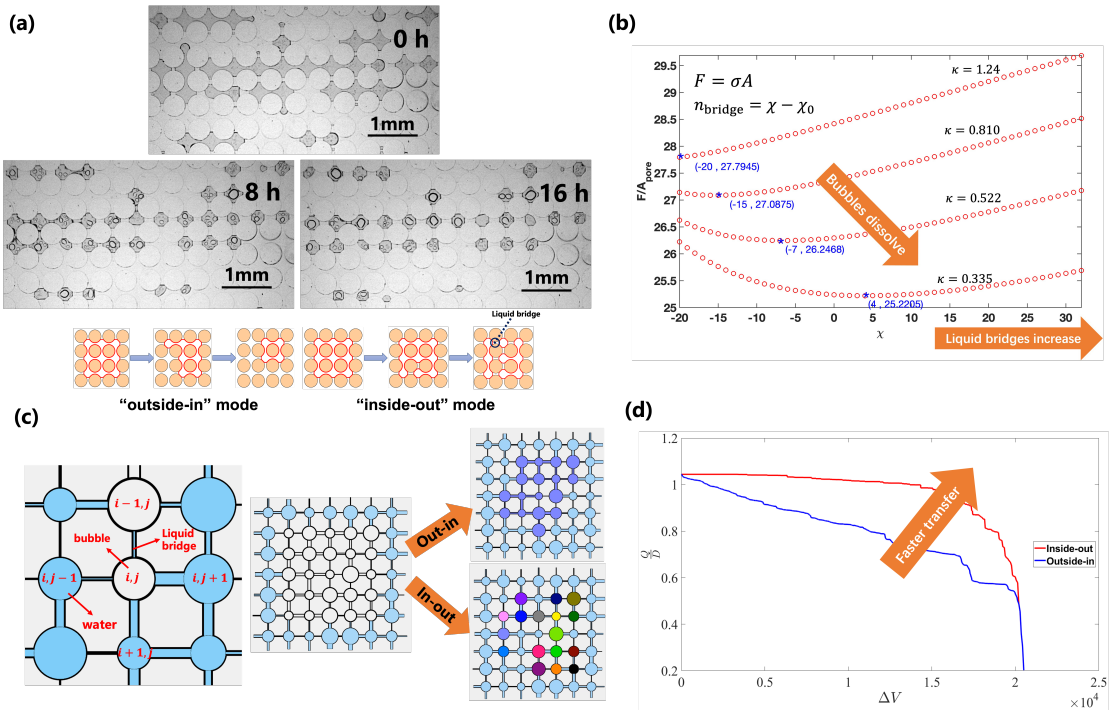

Figure 2: enter image description here

Figure 1 (a) Snapshots of experiment (above) and diagrams for 2 dissolution modes (below). (b) Free energy of ganglia with different curvatures changes with increasement of liquid bridges. (c) Diagrams for PNM and evolution of bubbles in two modes. Light blue represents water while the other different colors represent different bubble domains internally continuous but mutually isolated for liquid bridges. (d) Mass transfer rate changes through dissolution in different pathways.

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Poster / 248

Controllable generation of porous media hybrid multiple-point statistics and sliced Wasserstein metric

Author: Zhenchuan Ma[1]

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Porous media have a wide range of applications in various engineering fields. Accurate modeling microstructure of porous media is the basis for subsequent numerical analyses and structure–property relationship researches. Computational reconstruction methods play an important role in these studies, can address limitations of some imaging techniques that are difficult to directly model three-dimensional (3D) structures, such as 2D-to-3D microstructure reconstruction and specific structure generation, and provide a fast and efficient way to model microstructures. Current computational reconstruction methods include traditional methods and machine learning-based (or deep learning-based) methods. Compared with traditional methods, machine learning-based computational reconstruction methods show advantages in reconstruction accuracy and speed. However, such machine learning-based methods also have limitations in interpretability, controllability, generalization, and small data sample application, which make it difficult to deal with various reconstruction tasks. In the previous study, we developed a hybrid method combining multiple-point statistics and machine learning, which is capable of handling 2D-to-2D, 2D-to-3D, and 3D-to-3D reconstruction tasks. Whereas, there are still some limitations in dealing with controllable and conditional generation tasks.

To further improve the reconstruction performance, we propose a novel controllable generation method hybrid multiple-point statistics and sliced Wasserstein metric, design a controlled sampling strategy and a conditional reconstruction strategy, and make progresses in dealing with controllable and conditional generation tasks. In this method, multipoint statistical information is adopted for microstructure characterization and sliced Wasserstein metric and gradient optimization are used for microstructure reconstruction. The controlled sampling strategy enables microstructure generation for any given phase volume fraction, by sampling with purpose from multipoint statistical information of training images. While the conditional reconstruction strategy can generate different microstructures satisfying the condition data. In addition, the proposed method only requires a single data sample (a 2D image or a 3D structure) to complete the above tasks, which has advantages in controllability, generalization, and small sample data application. Finally, to verify the reconstruction performance of our method, multiple sets of experiments are performed on a variety of porous

media images (e.g., porous rocks, silica materials, battery electrode materials, and synthetic ceramics), by generating microstructures with different phase volume fractions and condition data from a single data sample. Comparisons of visualization, statistical parameters such as two-point probability function and linear path function, and numerical analysis are adopted to further show the effectiveness of our reconstruction results.

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MS11 / 249

Investigation of transport and deposition of micro-nano-bubbles in porous media using column test and microfluidics

Authors: Yazhou Cao[1]; Liming Hu[1]; Zhen-yu YIN[2]

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Micro-nano-bubbles (MNBs) enhanced oxidation presents a sustainable approach for contaminated groundwater remediation. Understanding MNBs transport and deposition in porous media is crucial for application and optimizing this technology. Firstly, the relationship between the number of MNBs and dissolved oxygen (DO) concentration was calibrated to provide a basis for the investigation of MNBs'migratory behaviors by employing DO concentration. Secondly, we developed a two-dimensional microfluidic model to simulate the pore structure of uniform-sized particles and directly observed the retention mechanisms of injected oxygen MNBs. The results indicated that MNBs retention predominantly occurs through surface deposition and hydrodynamic bridging, with no significant straining observed. Furthermore, we conducted one-dimensional column experiments using glass beads as porous media to examine the impact of porous media and groundwater chemical characteristics on MNB migration, deposition and re-mobilization. The findings revealed substantial MNB retention within the porous medium, with retention diminishing as the injection rate and glass bead size increased. Finally, the irregular quartz sand was employed in the column tests, which demonstrated a higher propensity for MNB capture comparing to uniformly-sized glass beads. Alterations in groundwater pH and salinity also influenced MNB migration by affecting the surface potential of both MNBs and the porous medium. In conclusion, this study provides a reference for further utilization of MNBs for remediation of contaminated groundwater.

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Poster / 250

Is it safe to continue relying on traditional porosity-permeability relationships?

Author: Mohammad Masoudi[1]

Co-authors: Mohammad Nooraiepour [2]; Hang Deng [3]; Helge Hellevang [4]

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The precipitation of secondary phases in porous media carries profound implications for the functionality and efficiency of diverse natural and engineered systems. This encompasses applications ranging from subsurface CO2 storage sites, geothermal systems, deep geological disposal repositories, tunnels, oil and gas reservoirs, to the treatment of contaminated groundwater. These precipitation processes alter the structure of porous media, reduce pore space, influence hydrodynamics, and even modify reaction rates by reshaping reactive surfaces. As a result, it becomes crucial to thoroughly investigate the hydrodynamic consequences of mineral precipitation in porous geometries. However, the prevailing practice of assessing the impact of precipitation reactions on flow and transport relies on simplistic permeability-porosity relationships. Commonly employed empirical, experimental, or theoretical models such as Kozeny-Carman, Verma-Pruess, and power law are favored for their convenience and simplicity. These models find widespread application in commercial or open-access simulators for diverse geo-energy and geo-environmental purposes. Nevertheless, our previous research has revealed that relying solely on such porosity-permeability relations introduces significant uncertainty. To address this knowledge gap and mitigate the associated uncertainty, we propose a hierarchical statistical approach to upscale the porosity-permeability relationship from the microscale to the macroscale. Our approach acknowledges the complexity of permeability-porosity evolution while still leveraging practical and readily available formulations. Simulations of the mineral precipitation process in diverse homogeneous and heterogeneous settings were conducted, and a power-law formulation for the porosity-permeability relation was fitted, resulting in a distribution of power-law parameters for each setting. This resulted in a lognormal probability distribution function (PDF) for all the cases. By incorporating this PDF into continuum scale simulations, a fit-for-purpose porosity-permeability relation is established, linking the microscopic dynamics of probabilistic nucleation and growth in porous media with the macroscopic application domain. For most objectives in reactive transport modeling, a three-step scheme adequately captures the pore-scale physics and dynamics, ensuring the representation of these properties at the application scale.

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The Impact of Water Saturation on Hydrogen Adsorption in Clay-rich Caprocks

Author: Mohammad Masoudi[1]

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Underground Hydrogen Storage (UHS) plays a pivotal role in the shift towards renewable energy resources, necessitating paramount attention to safety and efficiency. To maximize the recovery of stored hydrogen and ensure a reliable seal against leakage, it is crucial to comprehend the propensity for hydrogen migration through caprock. The migration may occur within the pore solution, where small H2 molecules can readily diffuse through pores and fractures of the seal. Accurate risk analysis requires a thorough assessment of hydrogen loss through the caprock, emphasizing the significance of hydrogen transport properties, including adsorption and diffusion. However, due to safety concerns surrounding hydrogen gas, comprehensive data on its interaction with various natural settings remains scarce. This study investigates the hydrogen adsorption of various natural and synthetic materials, including four shale samples from the Norwegian Continental Shelf and three standard clays. The samples underwent extensive characterization tests, such as X-ray Diffraction (XRD), X-ray Fluorescence (XRF), Scanning Electron Microscopy-Energy Dispersive Spectroscopy (SEM-EDS), and BET analysis. High-pressure gas adsorption analysis was conducted to measure hydrogen sorption isotherms. The experiments included dried and wet samples, with and without prior treatments. The results reveal that swelling clays, particularly those from the Smectite group, have a higher hydrogen uptake capacity. Additionally, when wet clay samples were examined, the presence of water resulted in competition between water and hydrogen for binding sites within the clay, leading to a decrease in hydrogen adsorption. The comprehensive testing and analysis conducted in this study provide valuable data for future risk assessments and enhance our understanding of geological hydrogen storage in various geological formations.

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MS13 / 252

Coupled mass and heat transfer model in porous media under high Knudsen number

Author: Shalong Xiong[1]

Co-authors: Nicole Vorhauer [2]; Petra Foerst [1]; Rui Wu [3]

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In the field of oil recovery and other industrial applications, the significance of an accurate and efficient model for porous media cannot be overstated. At present, most of the macroscopic models for the gas flow in porous media at a high Knudsen number are only investigated under pressure gradient. What's more, the thermal effect becomes prominent in a single tube as the rarefication degree increases whereby mass flow could occur in the direction of inverse temperature gradient, which is named as Transpiration flow. This phenomenon will surely make a difference in the mass transport and heat transfer process in porous media, leading us to determine the mass and heat transport coefficient in porous media under pressure gradient and temperature gradient, as the existing coefficients for mass transport are physically ambiguous and coefficients for heat transfer in porous media are not specified. Therefore, to fully reveal the transport mechanism in porous media under moderately high Knudsen numbers at a macroscopic scale, a novel approach is developed.

Specifically, the analytical solutions of velocity and heat flux to the Poiseuille flow and Transpiration flow in a cylindrical tube by the R13 moment method of rarefied gas theory are first obtained. Subsequently, they are separately incorporated into a three-dimensional pore network model that comprises thirty pores in each direction via newly derived mass flow conductivity and heat transfer conductivity in the form of Knudsen number. As a result, these pore network modellings derive the apparent permeability and the apparent Knudsen diffusion coefficient for mass flow and heat transfer under pressure gradient and temperature gradient respectively. It is found that the above four numerically computed properties fitted with the effective Knudsen number are consistent with their explicitly analytical form in a cylindrical tube. Hence, the analytical form of macro properties is then applied to the macro model for porous media simultaneously subjected to pressure gradient and temperature gradient. Also, a validation of the macro model is made by developing a heat and mass-coupled pore network model under the same boundary condition when the Knudsen number is under unity. To summarize, in this work, a computationally efficient and precise macro model for rarefied gas flow in porous media with the Knudsen number ranging from 0.001-1.0 is established.

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MS08 / **255**

Reactive Solute Transport in Heterogeneous Porous Media

Author: Mengzi Ren[1]

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CO2 geological storage in saline aquifer is significantly influenced by the reactive solute transport in the fracture media. However, the governing factors and coupling mechanisms of solute transport within the fracture at different periods under seepage-chemical coupling remain unknown. In this investigation, reactive solute transport experiment on sandstone fracture was conducted to determine the main mineral reactions. The fracture reactive solute transport analysis model taking mineral precipitation into account is proposed, and the fracture reactive solute transport characteristics under varying Pe number and Da number conditions are analyzed. The results of the dimensionless parameter analysis revealed that the Pe number was the governing factor of the solute transport process in the short period between injection and peak concentration of CO2, and that the time to peak solute concentration decreased with increasing Pe number. Under long periods of injection conditions, the solute transport process is governed by the Da number. Mineral precipitation at a high Da number obstructs the fracture, resulting in a progressive decrease in the variation rate of Ca2+ concentration during the late stage and the bypassing flow phenomenon of flow lines and species transport pathways.

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MS15 / **259**

Efficient 3D Digital Rock Detail Reconstruction and Quality Enhancement with Super-Resolution Transformer

Author: Zhihao Xing[1]

Co-author: Jun Yao [1]

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

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High-quality digital rocks are essential for high-precision pore-scale modeling. However, limited by the imaging hardware, meeting the requirements of high resolution (HR) and a wide field of view (FOV) simultaneously is challenging. In this study, we propose a novel Efficient Attention Super-Resolution Transformer (EAST) to boost digital rock quality, which reconstructs HR details from low resolution 3D images with wide FOV. To address the specific characteristics of digital rock tasks, EAST employs a hybrid loss function to recover sharp pore edges and combat noise. Furthermore, we utilize data augmentation techniques to improve model generalization. The hyperparameters of EAST are optimized to trade off speed and super-resolution quality. Through quantitative evaluations and qualitative visualizations, we validate the superior reliability of EAST in terms of recovering sharp edges and eliminating noise. Compared to the efficient convolutional neural network-based model RCAN, EAST achieves higher performance with only 22% of the parameters due to hybrid efficient attention mechanism. Finally, we verify the physical accuracy of the EAST reconstruction results by direct flow simulation method. The results demonstrate that EAST significantly reduces the relative error of single-phase permeability from 35% in Tricubic interpolation to 8%. Moreover, EAST is 185% faster than RCAN, which implies that EAST could process a digital rock with 10^9 voxels in 4.3 hours, thereby generating an impressive 6.4×10^{10} voxels.

Keywords: digital rock physics, 3D image super-resolution, deep learning, Transformer

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MS13 / 261

Pore aperture regulated surface adsorption and mass transfer of hydrocarbon and CO2 in organic nanopores

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Shale oil, widely distributed in organic (i.e., kerogen) nanopores, is playing an ever-increasing role in addressing the global energy crisis, but is faced with challenges of low recovery efficiency due to well-developed nanopores. It is believed that the pore size distribution of kerogen is in the range of several angstroms to tens of nanometers (AAPG bulletin 96 (6): 1099-1119). In such a narrow pore space, oil molecules are dominated by adsorbed phase, which is hard to recover relying on pressure drop (International Journal of Coal Geology 147 (2015): 9-24). CO2 huff-and-huff is identified as a promising method to enhance oil recovery while achieving CO2 sequestration. Clarifying the adsorption and extraction behaviors of hydrocarbons in kerogen nanopores is crucial for accurately predicting oil recovery and revealing CO2 enhanced oil recovery (CO2-EOR) mechanisms.
In this work, we adopted molecular dynamics (MD) simulation to study the static spatial distribution and dynamic mass transfer of hydrocarbon and CO2 in slit-shaped kerogen nanopores by carefully designing a series of pore apertures. It shows that the adsorption and extraction behaviors of oil molecules are closely related to pore aperture. Interestingly, we found that the surface adsorption of oil molecules demonstrates a non-monotonic trend of rising after falling as the pore size decreases. Specifically, when the pore size is reduced to a certain value, oil molecules exhibit a pseudo-double layer adsorption state, in which the surface adsorption peaks of oil molecules are significantly weakened. On the other hand, although the reduction of pore width adversely affects the extraction speed of oil during CO2 soaking, the recovery efficiency presents a jump for the oil at pseudo-double layer adsorption state. Meanwhile, the surface adsorption of CO2 is also greatly enhanced, which leads to the highest CO2/Oil ratio in the nanopores. Collectively, our work provides fresh and important insights into hydrocarbon occurrence state and CO2-EOR mechanisms in organic-rich shale reservoirs and builds up a good foundation for accurate predictions of oil recovery.

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Characterization of gas shale pore systems by porosimetry, pycnometry, surface area, and field emission scanning electron microscopy/transmission electron microscopy image analyses: Examples from the Barnett, Woodford, Haynesville, Marcellus, and Doig units. AAPG bulletin 96 (6): 1099-1119; Oil adsorption in shale nanopores and its effect on recoverable oil-in-place. International Journal of Coal Geology 147 (2015): 9-24.

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MS06-A / 262

Spontaneous Symmetry Breaking during Dispersed Fluid Flow through Porous Media

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Dispersed fluid systems (foam, emulsion, bubbly liquid, etc.) involves in many key geophysical/geochemical, environmental, and engineering processes[1-3]. However, regardless of many pore-scale and channel-scale approaches[4, 5], predicting dispersed fluid flow behavior in porous media is still a major challenge. Here we conduct experimental and theoretical investigation, trying to rationalize the long-puzzling gap between single-channel scale and porous media scale models for dispersed fluid flow.
We first conduct experiments in doublet microfluidic model (Fig. 1a). We fix Ca_d (dispersed fluid capillary number) and observe the flow state at varying Ca (total capillary number). At low *Ca*, very significant difference for blob fluxes between two parallel channels are identified even when the two channels are highly symmetric (Fig. 1b). After careful quantitative analysis, we realize that minor fabrication error cannot rationalize this symmetry breaking.
We thus hypothesize that this asymmetric flow of dispersed fluid is originated from a new symmetry breaking mechanism. We thus conduct stability analysis in a doublet system, that introduce an infinitesimal perturbation to assess its potential for self-amplification. Analysis shows that such symmetry breaking can emerge, if there is a negative correlation between pressure drop and total flow rate at a constant dispersed fluid flux ($\frac{\partial F}{\partial Ca}\big|_{Ca_d} < 0$) within a specific channel. The existence of $\frac{\partial F}{\partial Ca}\big|_{Ca_d} < 0$ correlation is successfully validated: theoretically, by classic Bretherton's correlation for non-viscous gas slug flow in a uniform cylindrical tube [6] (Fig. 1c); and experimentally, by microfluidic experiment along a single channel of sequential pore-throat structure (Fig. 1d).
This breaking of flow path symmetry, if emerges in porous media, may result in preferential flow even in homogeneous media. We conduct a demonstrative experiment in a homogeneous porous medium to validate the above inference. Surprisingly, we do observe significant non-uniform flow at steady state, as shown in Fig. 1e and Fig. 1f. Preferential paths carry almost all dispersed fluid flux, while blobs in other paths flow only occasionally and slowly. Noticeably, the dispersed fluid saturation is negatively correlated with its flux, which is contradictory against classic relative permeability idea, but can be well explained by the abovementioned spontaneous symmetry breaking.
This discovery of spontaneous symmetry breaking of dispersed fluid in porous media may bring new insight into the understanding and modeling of complex fluid behaviors in disordered geometry.

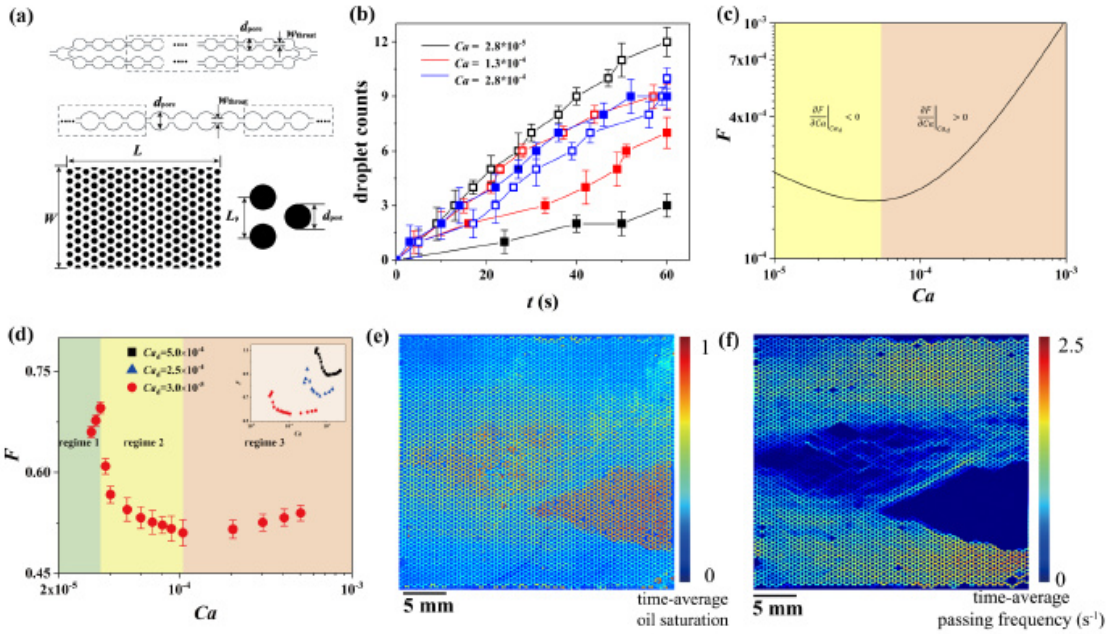

Figure 3: (a) The design of the doublet-channel model, single-channel model and homogeneous porous media model. (b) The experimental results of the cumulative number of droplets in doublet system for Cad = 1.5×10-5. Hollow symbols denote channel 1 results, while solid symbols represent channel 2 results. (c) Schematic diagram of F-Ca curve in a single channel for Bretherton model. (d) The experimental results of F-Ca curve along a single channel with Cad = 3.0×10-5 (in the main plot, and colors mark different regimes), and with Cad = 2.5×10-4 and 5.0×10-4 (in the inserted plotting). (e) Time-average dispersed fluid saturation map of the whole micromodel. (f) Time-average blob-passing frequency field map of the whole micromodel.

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Poster / 267

A multiscale simulation method for aerosol transport in a mouth-to-lobar bronchi model

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Prediction of aerosol deposition in the respiratory tract has become a major focus for inhaled drug delivery and air pollution prevention. Computational fluid-particle dynamics (CFPD) provides the most accurate local prediction results, but the computational cost is unbearable for the CFPD simulation of the whole respiratory tract. This challenge arises due to the multiscale nature of the respiratory tract and numerous bronchioles 1. A common practice is to truncate the bronchial tree and simulate on the truncated model using CFPD. In this study, a novel boundary condition for the truncated respiratory tract model based on multiscale simulation is proposed, named extended-bronchus-network (EBN) boundary condition. The truncated model is extended to the terminal bronchial and the air flow in the extended part is simulated using local hydraulic resistance equivalence pore network model (PNM) [2]. The pressure and flow rate at the outlet of truncated model is consistent with PNM, which provides the outlet boundary condition for CFPD of truncated model. A comparison against EBN with the widely used uniform pressure outlet boundary condition [3] is made. It reveals that EBN boundary condition in this study is more physiologically and closely to the clinical data. The maximum relative disparity of nano-micro aerosol penetration fraction of the right middle lobe and right lower lobe between these two methods is 93% and the maximum relative disparity of aerosol deposition fraction within the trachea-lobar bronchi is 30%. EBN boundary condition is implemented for the simulation of nano-micro particles transport in the mouth-to-lobar bronchi (MLB) model at the inspiration volume rate of 15, 60, 90 L/min, respectively. Result shows that for particles equal to or less than 1 μm in size, over 90% penetrate deeper into the pulmonary lobes, with inspiration volume rate and particle size having minimal impact on penetration fraction. However, micro particles more probably deposit in the MLB with larger inspiration volume rate. Notably, when particles larger than 6 μm are inhaled at 15 L/min or particles larger than 3 μm are inhaled at 60 L/min, over 40% of them deposit in the MLB. Particle deposition hotspots forming reason is qualitatively analyzed. This work provides a reference for the optimization of drug delivery, targeted therapy, the prevention and control of pollutants. It also lays a foundation for the simulation of aerosol transport in whole lung.

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Poster / 269

Microscopic damage rules of water flooding in ultra-low permeability reservoir: an experimental study based on the combination of microfluidic and low-field NMR technology

Authors: Yiping Wen[1]; Qi Li[1]; Jingyi Zhu[2]; Xinyu Tang[2]

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Water flooding is one of the important ways of oilfield development in China. However, due to the poor-compatibility between injected water and reservoir rocks and fluids, free particles such as inorganic scale and rock clay often block the pores and throats under the carry-over effect of water seepage, which leads to engineering problems such as water injection pressure increasing, underinjection of injection-wells and decreased oil production capability of production-wells. Conventional core experiments and numerical simulations were used to study the damage induced by water injection. Since the black-box nature of the core, researchers cannot observe the fluid flow rules in porous media, nor can they know the specific location and degree of core damage. Although the numerical simulation method can simulate the scale formation and the occurrence of scale particles, it ignores the real situation of scale particles being carried and moved by fluid, and can not obtain the real rules of water flooding damage to the reservoir.

Considering the shortcomings of previous studies, we combined low-field NMR and microfluidic techniques to explore the damage rules of injected water to the core of an ultra-low permeability reservoir in northwest of China. Firstly, low-field NMR online displacement technology was used to detect the signal intensity changes of the core along the axial direction, as well as the pores of various sizes during the water flooding process, and we obtained the injury rules of the core at different locations during the water flooding process. Further, we used μ-CT to scan the core slice and obtain its pore distribution information, and etched it on the glass chip for displacement experiment, and observed the damage rules of the scale particles generated by the combination of injected water and formation water on the porous media in real time.

It is found that free particles are selective to reservoir damage. Due to the low-resistance flow characteristic of fluid, free particles will be carried by fluid to the micro-fractures and large pores, causing greater damage. This kind of damage has mobile characteristics, free particles will be carried to the center and tail end of the core, and increase the blockage these parts over time. The microfluidic experiment further confirmed the rules obtained by low-field NMR method, and the accumulation of scale particles in the middle and rear of the chip was also found in the microfluidic displacement experiment. The particles size of these areas continues to increase, which increases the damage to the middle and rear of the reservoir, blocks the flow channel of the production wells, and seriously reduces the swept efficiency of the displacement phase.

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MS22 / 270

Nano Porous Particle: A Novel Additive for Gas Storage Technology Based on the Hydrate Method

Authors: Pengfei Wang[1]; Yinlong Li[1]; Ying Teng[2]; Hao Long[1]; Meng Han[1]

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This study investigates the thermodynamic and kinetic characteristics of nano porous particle as an additive in the formation of CH4 hydrate, essential for hydrate technology applications and energy estimation in gas storage process. Thermodynamic analyses were conducted with varying nano porous particle concentrations. Differential Scanning Calorimetry (DSC) was employed to determine phase equilibrium temperatures and pressures within the range of 3-10 MPa. As pressure increases, the endothermic peak shifts to the right, indicating higher decomposition temperatures, and the peak of hydrate decomposition intensifies, signifying enhanced hydrate formation with increased pressure. Phase equilibrium points measured by DSC align with existing literature values, indicating that nano porous particle does not alter CH4 hydrate phase equilibrium under varying pressure conditions.

The kinetics of CH4 hydrate formation were examined under different nano porous particle concentration. Observations show a reduction in the induction time with increased nano porous particle concentration, attributed to enhanced gas solubility and increased nucleation sites in the porous medium. The porosity, specific surface area, and mobility of nano porous particle accelerate hydrate formation and enable it to adsorb more CH4 than pure hydrate, emphasizing its role in gas storage. Raman spectroscopy was employed to analyze CH4 solubility in water with nano porous particle. Results demonstrate an increase in solubility with rising nano porous particle concentration, suggesting nano porous particle's significant role in promoting CH4 hydrate formation. This indicates potential efficiency improvement in CH4 hydrate production by substituting pure water with nano porous particle.

The stability of this nano porous particle immersed in water for various durations was analyzed by XRD and SEM, and the results were consistent without obvious structural changes. BET analysis confirms the stability of pore diameter and specific surface area. The good stability of nano porous particle can ensure the effectiveness of nano porous particle as an additive in the hydrate system.

In summary, this study reveals the thermodynamic, kinetic properties of CH4 hydrate formation in water with nano particles, providing insights into its potential applications and efficiency improvements in gas storage processes.

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MS09 / **272**

An Improved MCMP Pseudopotential Model for Immiscible Fluids Flow in Porous Media

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Extreme viscosity ratios emerge in many important applications such as carbon dioxide geological sequestration (CO2 is much less viscous than formation fluids), natural gas production and hydrogen storage (gas is much less viscous than water), and heavy oil reservoir recovery (oil is much more viscous than water). Clearly understanding the immiscible two-phase flow with extreme viscosity ratio can provide guidance for practical production.

Lattice Boltzmann method (LBM) has recently been widely applied for numerical simulation of pore-scale two-phase flow. However, prior LBM approaches on two phase porous media flow [1-4] present major limitation in modeling extreme viscosity ratio and low capillary number. It mainly stems from the large spurious currents[5,6] when dealing with multiphase flow problems in complex media due to insufficient isotropic, which results in poor stability and accuracy of the prevailing multiphase LB model. Consequently, genuine flow velocities, particularly under conditions of low capillary numbers or high viscosity ratios, become tainted with these unwarranted velocities. Such interferences significantly hinder a comprehensive understanding of two-phase flow mechanisms within porous media.

To address this challenge, we integrate interaction forces using a higher-order difference approach[7], building upon Porter et al.'s multi-relaxation MCMP pseudopotential model[8] with an explicit forcing format. Our findings point that adjustable parameters related to the non-conserved quantities within the multi-relaxation matrix offer a distinct advantage in diminishing spurious currents. Furthermore, by employing the color gradient model for the diffusive mixing of two-phase systems, we successfully achieve higher viscosity ratios. Notably, our improved model dramatically reduces maximum spurious currents in porous media by two orders of magnitude (from 1e-3 to 1e-5) compared to its predecessor. Based on this improvement, we simulate two-phase flow in porous media, spanning a broad capillary number range (4e-5 to 1e-2), extreme wetting conditions (0° to 180°), and high viscosity ratios (up to 100). We are therefore able to extract more accurate velocity distribution for diverse analysis on multiphase flow in porous media.

In general, we propose a novel MCMP pseudopotential model, that extends our capacity to numerically investigate immiscible fluid flow in porous media with low capillary number and extreme viscosity ratio flow.

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Poster / **274**

Simulation and Prediction of Natural Restoration for Arsenic-Contaminated Site

Author: ZOU Shengzhang[None]

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Contaminated soils typically possess self-healing capabilities, and the ecological concept of emphasizing natural restoration with supplementary artificial reinforcement has gained widespread acceptance. An investigation was conducted into the arsenic pollution status at an abandoned arsenic factory site in southern China. After identifying the spatial distribution characteristics of arsenic in the soil, indoor soil arsenic dissolution experiments were conducted under different conditions to obtain chemical kinetic parameters during desorption. A relationship model between desorption amount and time was established based on simulation results using Phreeqc. This model aims to predict the natural attenuation of soil arsenic based on natural restoration. The results indicate severe arsenic contamination in the original waste heap soil, with arsenic content reaching 181-283mg within 20cm below the surface in certain local areas. However, high concentrations of arsenic pollutants are mainly concentrated in the depth range of 30-60cm below the surface. This suggests that under the driving force of atmospheric precipitation, arsenic from the original waste heap infiltrates into the soil below the surface of 30-60cm. Due to the transformation of the soil from an oxidizing environment to a reducing environment, arsenic continuously accumulates, forming a relatively stable secondary pollution source that still poses a risk of groundwater contamination. The results of desorption simulation experiments using local normal rainfall and acid rain (pH=4.6) show that normal atmospheric precipitation can only desorb approximately 40.7% of the arsenic in the soil. It would take an additional 16.25 years to bring the arsenic concentration in the contaminated site to the second-level standard limit of soil environmental quality. Under acid rain conditions, the dissolution rate of arsenic can reach 65.4%, and considering the local annual acid rain rate, the arsenic concentration in the contaminated site can meet the second-level standard limit of soil environmental quality within 13.09 years.

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Poster / 276

Pore scale characteristics of CO2 trapping and oil recovery in heterogeneous layered sandstone

Author: Yingwen Li[None]

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The vertical variation in permeability is a typical heterogeneity of pore structure in sandstone reservoirs. We thus constructed a millimeter sized layered sandstone, and performed water-alternating-gas (WAG) injection and CO2 foam flooding. After each gas injection, the core was placed vertically for 24 hours and horizontally for 24 hours respectively to study the influence of gravity on fluid migration. The fluid distribution obtained by high-resolution X-ray microtomography indicates that layered heterogeneity leads to a large amount of oil being trapped in the low-permeability layer. Although the WAG strategy improves the oil recovery of layered porous media, a large amount of oil is still trapped in low-permeability layers after two WAG cycles. After CO2 foam flooding, the oil in the low-permeability layer can be effectively recovered. During the no-injection period, the difference in fluid density caused fluid migration and crossflow, that is, the oil in the low-permeability layer decreased while the oil in the high permeability layer increased, which is beneficial for subsequent oil production. Increasing the number of WAG cycles is beneficial for improving the CO2 capillary trapping efficiency. The relative permeability of CO2 in low-permeability layers is relatively low, with residual gas mainly distributed in single pores. CO2 clusters in the low-permeability layer have a large surface area to volume ratio, thus the CO2 capillary trapping is more stable, and the amount of CO2 dissolution trapping will be greater.

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Poster / 277

Direct Pore-Scale Simulation of the Effect of Wettability Alteration by Low-Salinity on Oil Mobilization in 3D Natural Sandstone

Author: Haoyun Li[1]

Co-author: Yongfei Yang [1]

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Wettability is an important factor controlling the pore-filling mechanism and displacement efficiency in the subsurface pore space. The trapped phase can be mobilized by wetting alteration, which is one of the main mechanisms of enhanced oil recovery technologies, such as surfactant flooding and low-salinity water flooding. Despite recent advances in the simulation of wetting alteration at the core scale or beyond, there are very few works that have modeled the wettability alteration at the pore scale, especially in three-dimensional (3D) micro-CT images, causing fluid displacement and retrapping mechanisms during wettability alteration are not well understood. With this objective, a wettability alteration model by low-salinity is developed and implemented in the open-source computational fluid dynamics software OpenFOAM (Open Source Field Operation and Manipulation), where both the Navier-Stokes equations for oil/water two-phase flow and the advection-diffusion equation for species transport are solved. The proposed model is validated against a published sinusoidal channel micromodel and then applied to 3D micro-CT images of sandstone to investigate the interplay between wettability alteration and pore structure. This study takes into account the effect of initial wettability, different degrees of wettability alteration, different time scales of wettability alteration, and different injection scenarios on oil trapping and the ultimate oil recovery factor. A larger degree of wettability alteration results in a higher oil recovery factor during tertiary low salinity water flooding. However, the oil recovery factor will first increase and then decrease with the increase of wettability alteration degree due to the snap-off effect during secondary low salinity waterflooding. In tertiary low salinity waterflooding, a lower wettability alteration time scale under the same degree of wetting alteration produces more oil. This study emphasizes the important interplay between wettability alteration, pore structure, and time scale during low salinity water flooding, and can explain some observations in recent micro CT experiments.

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MS16 / **278**

Unveiling moisture transport mechanisms (vapor vs. bound water) in cellulosic materials: application to droplet absorption

Author: Yuliang ZOU[1]

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Thin cellulosic materials such as natural textiles, paper, or bio-based walls, exhibit a remarkable capacity to absorb humidity from the environment through "bound water" sorption within nanopores, constituting up to 30% of their dry mass 1. Understanding the mechanisms of induced water transfers is crucial for advancing industrial processes and sustainable practices across various fields, including wood drying, paper production and usage, moisture transfers in clothes or hair, and humidity regulation of bio-based construction materials. Despite the significance of this knowledge, the transport and storage mechanisms of moisture in these materials is still poorly understood, often relying on modeling assumptions of dominant vapor transport with an assigned diffusion coefficient [2].
Our research addresses this research gap by highlighting the critical role of bound water transport within interconnected fiber networks. Particularly, at low porosity, our findings reveal that bound water diffusion surpasses vapor diffusion [3]. Through rigorous experimentation, we isolate diffusion processes and derive diffusion coefficients, establishing a comprehensive model for moisture transfer. Remarkably, our model accurately predicts the spatial distribution evolution of bound water over time across varying porosities, as confirmed through Magnetic Resonance Imaging (MRI). This paradigm shift, indicating the dominance of bound water transport over vapor transport, provides control of humidity-related processes.
Furthermore, our observations extend to the essential role of bound water diffusion in the fate of an aqueous droplet over long time, specifically in papers and masks. From Magnetic Resonance Images, it appears that even in a close container blocking evaporation the liquid water of this droplet reaching a non-treated cellulosic sample, progressively disappears. We show that our model fully describes this process: the free water is rapidly absorbed as bound water which then diffuses through fiber network partly as bound water and partly as vapor.

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MS01 / 280

Pore Storage for Green Hydrogen: A Sensitivity Analysis of Geological Parameters at Ketzin Anticline (Germany)

Author: Lea Döpp[1]

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The increasing demand for green hydrogen in Europe, particularly in Germany, requires extensive storage capacities to compensate the imbalance between production and consumption. Although salt caverns are known as safe and reliable medium for large scale hydrogen storage, however, these are geographically limited. Therefore, porous reservoirs - such as saline aquifers and depleted hydrocarbon fields - are suggested as alternative solutions.

This study investigates the preliminary feasibility of underground hydrogen storage in Ketzin, Brandenburg, Germany. The Ketzin site was already used for the storage of town gas, natural gas and CO2 as well in the past decades. The potential hydrogen storage unit is the Stuttgart formation, which exhibits fluvial facies characterized by channel and floodplain elements. In this study, we consider a homogenous model for a sensitivity analysis, where porosity, permeability, capillary pressure, relative permeability, hydrodynamic dispersivity as well as salinity of the brine are investigated within their known ranges. The effect of geological parameters is analysed with respect to storage performance such as gas injectivity and productivity as well as sustainability derived from long-term injectivity and productivity.

The results from the sensitivity study reveal that changes in capillary pressure and permeability exhibit the most significant influence on productivity, with variations of up to 150% observed in both positive and negative directions. The sustainability, on the other hand, is significantly negatively influenced by low porosity, low permeability as well as high dispersivity by up to 80 %. However, the results of the high salinity of the water solution have the most positive influence on this index.

The analysis not only holds significant importance in advancing fundamental knowledge on the storage of hydrogen in porous reservoirs and its influencing parameters. It also provides a solid starting point for the systematic evaluation of the feasibility of a prospective regional hydrogen demonstrator. Future work will be carried out with a more complex model including the lithological heterogeneity and focus on the optimization of the operating parameters like the duration of cushion gas injection and storage cycles as well as the injectivity and productivity.

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MS22 / 281

Experimental Study and Process Modeling of Closed-loop LIB Recycling with Lithium Sulphate Electrodialysis

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Lithium-ion batteries (LIBs) play a crucial role in urbanization and human life, providing essential energy storage capabilities distinguished by their high energy density, long cycle life, and low weight [1,2]. The hydrometallurgical method for recycling of spent LIBs is of great importance due to its remarkable features, including high metal recovery rates, their capacity for Li+ and Al3+ recycling, extraction of high-purity metals, operation at relatively low temperatures, and reduced energy consumption and emissions [3,4]. The conventional hydrometallurgical processes generate a sodium-enriched wastewater, requiring treatment prior to safe discharge. This study concentrates on a closed-loop recycling process for spent Lithium Nickel Manganese Cobalt Oxide (NMC) cathode material, depicted in Fig. 1. This innovative approach also aims to eliminate sodium ions through the deviation from conventional hydrometallurgical methods, concurrently repurposing dissolved ions within the disposal slurry, resulting in a more eco-friendly and cost-effective approach. Lithium hydroxide (LiOH) is utilized as the precipitating reagent in this process, while lithium recovery is conducted employing electrodialysis (ED) to regenerate LiOH and sulfuric acid (H2SO4) from the lithium sulfate solution. A portion of the LiOH and H2SO4 reagents is subsequently employed in the leaching and precipitation steps, establishing a closed-loop recycling system. To validate this approach, an experimental setup was established to study leaching, impurity removal, and metal extraction processes. The closed-loop recycling process was further investigated by the simulation of this process using Aspen Plus. Therefore, the Aspen Custom Modeler was employed to create the ED module in both continuous and batch configurations. Subsequently, this ED module was incorporated into Aspen Plus to integrate with the recycling process under experimental operational conditions. The minimal deviations of 3.34% and 2.38% within the precipitation and co-precipitation processes indicated the accuracy and validity of this work. Continuous and batch-mode EDs were integrated with the recycling LIBs process to extract LiOH and H2SO4 from the Li2SO4 solution resulting from the metal extraction procedure. Based on the results, a 40% greater recovery of LiOH solution from the Li2SO4 solution using batch-mode ED indicates the better performance of this mode compared to continuous configuration. The effect of time and temperature on the leaching efficiency is also investigated. As illustrated in Fig. 2, it was found that the enhancement of reaction time from 5 to 30 min resulted in the 33, 39, 45, and 73% increment on Li+, Ni2+, Co2+, and Mn2+ leaching efficiency, receptively. Also, the 53% increment of Li+ was observed by raising the temperature from 10 to 70℃.

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Poster / 282

Analyzing Impacts of Gas Evolution within a Batch-Mode Electrodialysis of Lithium Sulfate using Two-Phase Flow CFD Simulation

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Electrodialysis (ED) technology relies on the selective permeability of ion exchange membranes, which allows for the separation of ions in a solution under the influence of an electric field [1,2]. ED has been frequently used for recovery of acids and bases [3,4]. Due to the growing demand for electric vehicles and the crucial need for recycling the lithium-ion batteries (LIBs), this study investigates the ED of Li2SO4 solution, aimed at comprehending the efficacy and requisite control measures for effective closed-loop recycling of spent LIBs. The enhanced flexibility and energy efficiency of batch-mode EDs highlight the significance of time-dependent models. The gaseous molecules evolved from electrochemical reactions induce localized turbulence, significantly impacting the velocity, potential, and concentration distributions. This study presents a two-phase model that analyzes the dynamic behavior of a batch-mode Li2SO4 ED and investigates the bubbles'impact employing an Euler-Euler model. The finite element method solves time-dependent hydrodynamic, mass conservation, and electrochemical equations. The excellent agreement between the model and experimental data shows the accuracy and validity of this model, emphasizing its applicability to analogous electrochemical processes such as electrolysis. According to the results of this two-phase flow model, the maximum volume fraction of H2 and O2 bubbles at the surface of the cathode and anode are 9% and 5%, respectively. As illustrated in Fig. 1, It is observed that the buoyant and drag forces induced by bubbles lead to a significant increment in liquid velocity and circulation of electrolyte solutions in concentrate channels. The bubble-induced turbulence disrupts the uniform velocity distribution near electrodes and increases the liquid velocity magnitude. This circulation of electrolyte solution declines the average concentration polarization across IEMs and increases ionic fluxes, particularly on the concentrate side of IEMs, which leads to the improvement of ED performance, as observed in Fig. 2. The liquid circulation leads to a substantial 60% reduction in the average Li+ concentration polarization across the CEM. In this case, the average total Li+ flux enhances by 12%, resulting in the significant increment of average Li+ concentration from 551 mol•m-3 to 768 mol•m-3 at t=2 hours. Furthermore, the enhancement of current density and reduction of bubbles diameter results in the increment of gas volume fraction. Increasing the flowrate causes a decrease in the average gas volume fraction and eliminates the impact of bubbles on the liquid velocity, as shown in Fig. 3. The effect of bubbles on ohmic overpotential is also discussed, and it is understood that it is highly dependent on inlet flowrate and liquid circulation. The presence of bubbles increases the ohmic overpotential by approximately 0.5 V in high inlet flowrate, F_in=0.3 L•s-1, that no circulation is observed. However, when electrolyte solutions circulate at low inlet flowrates, F_in=0.03 L•s-1, a higher ionic concentration and consequently lowers ohmic overpotential of electrolyte solutions are observed.

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MS01 / 284

Investigating multiphase flow dynamics in rock fractures via XCT imaging for hydrogen storage optimization

Authors: Sojwal Manoorkar[1]; Soetkin Barbaix[1]; Hamdi Omar[1]; Dominique Ceursters[2]; Steven Colpin[2]; Maxime Lathinis[2]; Tom Bultreys[1]

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The global climate change crisis has heightened the current focus on sustainable energy solutions, where hydrogen has emerged as a promising candidate for clean and efficient energy storage. However, effective and scalable storage of hydrogen remains a major challenge. Underground rock formations, including fractured reservoirs, offer a potentially impactful solution for hydrogen storage. This research investigates multiphase flow dynamics within rock fractures to optimize hydrogen storage strategies. We focus on a karstic aquifer formation currently used to store natural gas in Loenhout, Belgium. Leveraging state-of-the-art X-ray micro-computed tomography (XCT) imaging, we study the dynamic behavior of gas displacing the brine within intricate networks of rock fractures.

We employ core flooding experiments coupled with XCT imaging to investigate the pore-scale dynamics of drainage and imbibition in rock fractures. Recognizing the challenges of sampling natural fractures, we induce artificial fractures in samples with low initial permeability from the Loenhout formation, using the Brazilian tensile test method. The experiments are conducted on mm-scale cores featuring fractures with a size on the order of 102 microns, allowing us to capture intricate flow features at a resolution of 6 microns. The study involves the injection of three different gases; hydrogen, methane, and a hydrogen-methane mixture—through brine-saturated fractures.

We analyse the fluid distribution and differential pressure response throughout drainage and imbibition at two different capillary numbers. This research methodology integrates advanced image processing and computational fluid dynamics simulations to extract quantitative data from the XCT images. This approach facilitates a nuanced understanding of gas transport mechanisms, capillary pressure effects, and the influence of fracture characteristics on multiphase flow dynamics under varying gas compositions.

Preliminary results offer insights into fracture permeability, aperture distribution, and the impact of geological heterogeneity on hydrogen migration. The study also aims to highlight the impact of different gases on preferential flow paths within fractures, thereby influencing the spatial distribution and storage efficiency of hydrogen and methane .

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Poster / 286

Investigating Hydrogen Storage in Pore Media of Saline Aquifers: A Numerical Study on Wettability and Pore Structure Impact

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Hydrogen, as a promising clean energy source, holds significant potential for energy transition and the efficient utilization of clean energy. However, large-scale hydrogen storage poses a limitation to its large-scale utilization and further development. Saline aquifers, characterized by favorable pore space and temperature-pressure conditions, are considered promising candidates for large-scale hydrogen storage. Therefore, our study focuses on investigating the flow of hydrogen in porous sandstone media during the initial injection and extraction process.
Utilizing the volume of fluid method, we conducted direct numerical simulations of this process, scrutinizing the impact of wettability, capillary number, and pore structure on hydrogen flow, storage capacity, and loss rate. The result reveals that hydrogen flow in underground porous media is predominantly governed by capillary forces, with hydrogen primarily stored in larger pores and channels. Increasing hydrogen wettability enhances reservoir storage capacity but concurrently results in elevated residual hydrogen after the extraction process. Regardless of reservoir wettability, hydrogen losses during the initial injection and extraction process are significant. Reservoirs characterized by larger pore and throat radii exhibit higher effective hydrogen storage capacity. Additionally, reservoirs featuring higher coordination numbers and enhanced connectivity contribute to greater hydrogen storage capacity and improved recovery rates.

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MS10 / **287**

Inverse gas chromatography, a new technique for correlating surface energy porous media to saturation

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Multiphase flow and reactive transport in porous media play a key role in various applications needed for establishing hydrogen as an alternative energy carrier. To successfully establish hydrogen, the porous media facilitating the hydrogen flow in presence of another fluid, needs to be optimized in terms of reactivity and transport properties. Two important parameters controlling reactivity and multiphase flow transport in a porous medium are surface area and surface energies of porous media surface in relation to saturation. In this study, inverse gas chromatography (iGC) is proposed to simultaneously measure surface energy distribution and surface areas of porous media in correlation to saturation.

Inverse gas chromatography (iGC) is a powerful, sensitive, and relatively fast technique for characterizing the physicochemical properties of porous media such as BET surface area and surface energy distribution 1. In this technique, a single gas, known as probe molecules, is injected into a column packed with the porous sample under investigation. The probe molecules pass through the column, interact with the porous material, and the retention time of the probe molecules is measured at the end of the column. Measuring the retention time for different probes, e.g. polar and non-polar, enables us to determine a wide range of physicochemical properties of the porous material. Recent advances in commercial IGC enable users to perform the iGC measurements at different controlled humidity. Due to the capillary condensation, different relative humidity can create wide range of saturation. By performing classical iGC experiments in these conditions, surface energy distribution and surface area of sample, for the first time, can be correlated to saturation under same experimental conditions. Depending on the degree of hydrophilicity of the sample, water follows different adsorption/saturation mechanisms as relative humidity of experiments increases. In the following paragraph, the expected results of iGC measurements on Teflon samples, representing hydrophobic situation, is discussed.

The water molecules' presence in the system initially adsorb on surface high-energy sites, i.e. polar functional group or cracks on the surface, and then as the relative humidity of experiments increases, based on the competition between cohesive and adhesive forces, water adsorption would continue on either the surface or the initial adsorbed molecules to form clusters [2,3]. In the case of the hydrophobic sample, the water saturation mechanism follows the latter scenario. In this stage, a decrease in polar component of the surface energy is expected (shown in Figure 2). The increase in size clusters as RH increases would result in a slow decrease in measured dispersive component and BET surface area. Clusters continue to grow until they reach to critical size when first stable nanodroplets can form on the surface. The formation of nanodroplets will cause an abrupt decrease in BET surface area and, conversely, increase in the polar component of surface energy due to the formation of stable water surface. As the RH of experiments increases, nanodroplets start to merge and slowly cover the surface, which results in a further decrease in surface area and a slow decrease in surface energy components.

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MS06-A / 288

Direct imaging of surfactant/polymer floods in sandstone cores utilising a combined PET/ X-ray CT approach

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With the ongoing transition towards net-zero, focus has been gradually shifting away from exploration and into the maximisation of production from already existing reservoirs. Here, traditional oil recovery methods typically extract around 30% of the oil in place –giving large opportunity for more efficient recovery techniques. Among which, surfactant/polymer methods have the capability of increasing recovery up to 70% by both liberating trapped oil and improving the displacement efficiency.

However, the relatively high cost of the surfactant is a major concern and, as such, ensuring its efficient and maximum utilisation is pivotal to a successful operation. To this end, methods are needed to understand the mixing process within the surfactant/polymer slug. Traditional approaches use a surfactant effluent breakthrough curve, but the results are associated with significant uncertainty due to the complexity of the flow dynamics present within a surfactant/polymer flood, with the formation of an oil bank and sharp saturation fronts. As such, extrapolation to in-situ behaviour remains a major challenge.

In this work we present results from a coupled experiment employing both PET and X-ray CT as imaging techniques aimed at the direct visualisation of both saturation profiles (by X-ray CT) and tracer propagation within a surfactant/polymer flood (by PET). The overall experiment consisted of two identical surfactant/polymer corefloods –conducted on Bentheimer –with the individual imaging techniques applied independently. Both experiments employed surfactant/polymer flooding as a tertiary recovery method –following a waterflood. The flooding scheme consisted of a 0.7 PV surfactant/polymer slug (L-145-10s 90/HPAM) followed by a 0.5 PV polymer slug (HPAM) to displace the residually trapped oleic phase (decane). For the PET experiment, two radiotracer pulses (FDG) were injected at the front and rear of the surfactant/polymer slug to investigate the mixing dynamics within the slug.

Via the use of X-ray CT, and the visualisation of the saturation profiles, the chosen combination of flooding regime and fluids was shown to both increase recovery, up to 86%, and form an oil bank – characteristic of a surfactant-based displacement process. Via the use of PET, the concentration profiles of the injected tracer pulses were reconstructed in up to three-dimensions as they progressed through the core. Mixing indices, such as the dilution index, spreading length and segregation index, were computed and compared to available single phase tracer experiments conducted on Bentheimer and other rock samples of varying heterogeneity. Notably, the calculated indices indicate comparatively enhanced mixing for Bentheimer –with behaviour mimicking that of more heterogenous systems. Lastly, via the combination the two imaging techniques, qualitative observations regarding the influence of the saturation fronts on the shape of the tracer concentration profiles was made. Overall, through this work, we demonstrate the feasibility of utilising PET in more complex flooding environments to investigate mixing, but also highlight the complementary nature of X-ray CT and PET as imaging methods.

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MS06-B / 290

Wettability acoustic probing in granular porous media

Authors: Yangpu Chen[1]; Li-Yun Fu[1]; Tobias Mueller[None]

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Surface wettability determines the property of a solid surface in contact with a fluid. It plays a major role in reservoir engineering applications involving fluid transport phenomena. For example, it is critical to hydrocarbon recovery where wettability not only influences the sweep efficiency, but also influences the remaining oil distribution. Since the wettability tends to affect the mechanical properties of rocks, it provides a potential means to remotely monitor the movement of spilled nonaqueous phase liquids in the subsurface via acoustic monitoring. However, there is a lack of direct wettability measurement conditions in underground applications. As widely utilized methods in geophysical exploration, borehole sonic logging and seismic surveys could be used as a potential far-field probing tool for wettability changes. Understanding the acoustic response to wettability changes becomes crucial for this purpose.

To generate a favorable experimental condition for wettability acoustic monitoring, we establish an ultrasonic experimental basis for observing changes between hydrophilic and weakly hydrophilic conditions in (partially) saturated granular porous media. Glass beads are employed to construct granular porous media with fully interconnected pores and are chemical-treated to alternate the wettability condition. Particular attention is paid to ensure the uniform distribution of water across bead packings at different saturation levels, aiming to diminish the impact of patchy water distribution.

The P- and S-wave velocities and attenuations are measured with increasing saturation for the bead packings before and after chemical treatment, respectively. The results illustrate that the chemical treatment increases contact angles and improves the water–bead coupling, leading to higher velocity and lower attenuation of coherent waves. The Gassmann-Wood-Walton model predicts the behavior of coherent waves under different wettability conditions assuming a change in the coordination number. Once reaching a critical saturation, incoherent high-frequency waves are developed with higher propagating velocities. The treatment reduces the amplitude of these incoherent waves to some degree, probably due to the improvement of water–bead coupling. We interpret the observed incoherent waves in terms of the wettability-dependent ability for water to bridge neighboring beads. The velocity of incoherent waves is exceeding the Gassmann-Wood prediction at partial saturation but is close to the fully water-saturated condition. This is suggestive of a propagation path of incoherent pulses resembling the fully water-saturated condition. In our interpretation, this is because the presence of a critical amount of water creates a favorable and wettability-dependent condition to form liquid bridges connecting neighboring grains.

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MS09 / 291

Identification and assessment of three-phase boundaries in porous electrodes of solid-oxide electrolysis cells based on a 3D microstructure model

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Hydrogen energy is regarded as a promising energy carrier due to its high energy density and non-pollution. Solid oxide electrolysis cells (SOECs) have been studied extensively as a promising way for massive hydrogen production from renewable but unstable energy sources. The electrode microstructure of SOECs has a significant influence on their electrochemical performance. To better understand the relationship between their microstructures and electrochemical performance, the quantification of key microstructural parameters such as the three-phase boundary (TPB) density and phase connectivity are required. The density and activity of the TPB sites are crucial in determining the electrochemical performance of SOEC electrodes. Therefore, it is also important to find the quantitative relationships between the active TPB density and electrochemical performance. Many efforts in microstructural analyses of SOEC electrodes via focused ion beam-scanning electron microscopy (FIB-SEM) have provided a great opportunity to link the microstructural properties to the electrode performance and the active TPB density is usually evaluated from geometrical models. However, due to the influence of conductivity and mass transfer of the gas phase, not all TPB identified from the geometric models are electrochemically active. Also, it is hard to quantitively calculate the active TPB density linking to the charge transfer. Here, we developed a comprehensive method to distinguish the active and inactive TPB which combined the image-based method and finite-element (FE)-based method. A 3D pore-scale model based on the real three phases and TPB lines was built to capture mass transfer, electron/ion transfer, and electrochemical reaction processes. The TPB sites were assessed with their contributions to the total current of the electrodes. By comparing the active TPB densities calculated from geometrical models (image-based method) and that of the developed model in this study (combined image and FE method), the proposed model was more accurate in predicting electrode electrochemical performance. This provides an effective way to reduce experimental costs and time but also deepens our understanding of the microstructure of porous SOEC electrodes.

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MS10 / **293**

Darcy-Scale Image Analysis for laboratory CO2 storage and fracture flow

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Imaging has always played a vital role in obtaining a better understanding of porous media processes through laboratory experiments. In contrast to pore-scale imaging, extracting Darcy-scale interpretation from porous media experiments has so far not drawn equally big attention. On the other hand, various imaging techniques used in the lab often do not offer pore-scale resolution, e.g., CT-PET, MRI, or optical images. Targeting the dedicated processing of image data from aforementioned sources in a unified way, a new software package has been developed to enable both qualitative and quantitative research based on experimental data: DarSIA (short for Darcy-Scale Image Analysis) 1. It provides unified input capabilities for various data types as well as a range of preprocessing tools, upscaling routines, and multi-image comparison tools allow for direct comparison. To mention two examples, such include tools to e.g. quantify the pointwise mechanical deformation in terms of a displacement map; and measure the disparity between two fluid configurations in terms of Wasserstein metrics and associated optimal transportation maps. Moreover, DarSIA provides I/O for simulation data formats and thus conventiently allows for bridging computational and experimental research.

In this talk, we present the philosophy behind DarSIA, and showcase its application for two example studies:

1. the evaluation of optical image series of laboratory CO2 storage for the FluidFlower Validation Benchmark Study for the Storage of CO2 [2,3],
2. comparison of PET images of flow in fractured media against simulation data in the context of a validation study for mixed-dimensional modeling [4].

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MS01 / 296

Microstructural heterogeneity and alteration of reservoir sandstones with experimental exposure to hydrogen

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Co-authors: Christopher Rochelle [2]; Edward Hough [2]; Kevin Taylor [3]; Lin Ma [3]

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Energy storage is becoming an increasing concern as the world transitions towards unpredictable renewable energy production. Hydrogen is expected be a key player as it can be produced through electrolysis of water using renewable electricity and used as a clean energy carrier to decarbonise industry, hence hydrogen storage is energy storage. Its small molecule size and low density means large-scale storage (TWh) is only feasible in the subsurface, such as porous reservoirs of saline aquifers. These are stratigraphically and geographically widespread globally. Porous storage of hydrogen is yet to be implemented, hence the influence of injected hydrogen on the subsurface under reservoir conditions (elevated temperatures and pressures) remains unknown. This includes geochemical reactions instigated from interactions between minerals, pore-fluid, and hydrogen within rock microstructure. It is essential that containment of hydrogen in porous rocks is proven prior to implementation, and that reservoir behaviour is comprehensively understood. As hydrogen must remain in the reservoir as expected and be recoverable in high volumes and purity.

This study relates to a larger collaboration between the British Geological Survey, Industrial Decarbonisation Research and Innovation Centre, and the University of Manchester. That provides lab-based microstructural characterisation and assessment of changes in reservoir rock properties caused by exposure to hydrogen in batch-reactor experiments under reservoir conditions (50oC & 150 bar). Reservoir rocks analysed are considered representative of possible targets for onshore hydrogen storage in the UK (Sherwood Sandstone and Lower Greensand reservoirs). Samples were thoroughly characterised pre- and post- experiment through a multitude of multi-scale imaging and measurement techniques, with a particular focus on x-ray computed tomography to reveal internal structure non-destructively. This exposed the microstructural heterogeneity within sandstone reservoirs, as well as microstructural alteration following hydrogen exposure. Sherwood Sandstone samples, although compositionally similar, exhibit two prominent textures. Channel-base with moderately sorted grains and a restricted pore network containing preferential alignment (porosity 8.95%; mean pore size 41.54μm). And the more dominant channel-fill, also moderately sorted but the pore-network is well-connected (porosity 24.47%; mean pore size 187.33μm). Lower Greensand samples have extremely variable microstructure and composition dependent on sample formation. Hythe Formation is well-sorted with a well-connected pore network (porosity 28.42%; mean pore size 174.90μm) dominated by quartz, glauconite, and muscovite. Instead, the Sandgate Formation is poorly sorted with a restricted pore network (porosity is much lower 15.34% and mean pore size 36.36μm) and is composed of quartz, calcite, and feldspar.

Overall, no major changes to rock microstructure or composition were observed following hydrogen exposure. This is important as it suggests the reservoir investigated are safe for hydrogen storage, which is promising for the UK. However, the migration of a fine particle was seen within one sample. The experimental design may have influenced other minor changes observed, such as grain loss around the edges of samples. Although no conclusive alterations have been seen in the results of these experiments, it remains possible that geochemical reactions will occur in reservoir compositions containing more reactive minerals, such as those rich in pyrite and anhydrite. Hence further investigation is required.

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MS15 / 298

Machine Learning Assisted Numerical simulation of Propylene Glycol-mixed Steam Enhanced Extraction in Unsaturated soils

Authors: Zhixin Chen[1]; Yue Wang[2]; Holger Class[2]; Rainer Helmig[2]; Liming Hu[1]

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Contaminated soils with hazardous persistent organic pollutants, such as Polycyclic Aromatic Hydrocarbons (PAHs), present significant challenges for efficient remediation, attributable to their low mobility and bioavailability. The technique of Propylene Glycol (PG)-mixed steam enhanced extraction has emerged as a promising remediation technology, markedly increasing the solubilization and desorption of PAHs through the application of condensed PG and input enthalpy. Despite its potential, a comprehensive understanding of the heat and mass transfer dynamics during PG-mixed steam injection remains conspicuously underexplored, a gap critical to determining the technology's remediation scope and efficacy. In this study, a compositional two-phase flow model was constructed to elucidate the heat and mass transfer mechanisms in unsaturated soils subjected to PG-mixed steam injection, utilizing the Dumux framework. To account for the chemical equilibrium of water, PG, and air across both gas and liquid phases, the 'feos' toolbox was employed for phase equilibrium and thermodynamic property calculations, enabling the determination of the fugacity coefficients for the various components in the liquid phase. Simultaneously, the behavior of gas-phase components was modeled as an ideal gas. A multi-layer neural network was developed and trained to predict the fugacity coefficients of these components under diverse conditions, including variations in temperature, pressure, and liquid-phase composition. This model serves as a novel approach to provide fugacity coefficients, facilitating the computation of the mole fraction of each component in both phases. Comparative results indicate that the machine learning model substantially enhances computational efficiency relative to tabulated searches for fugacity coefficients. The model yields plausible predictions of temperature and pressure variations, as well as the distribution of water and PG across both phases, surpassing the traditional assumption of an ideal PG-water solution. Subsequent sensitivity analysis will delineate pivotal parameters governing heat and mass transfer during PG-mixed steam injection, identifying critical operational zones. Overall, this numerical model is instrumental in advancing the understanding of PG-mixed steam enhanced extraction processes and serves as a foundational reference for engineering design.

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MS08 / **299**

How does access to continuous brine sources in saline aquifers enhance salt precipitation dynamics during geological CO2 storage?

Author: Mohammad Nooraiepour[1]

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Meeting the long-term expectations of Carbon Capture and Storage (CCS) technology hinges on injecting massive volumes of CO2 annually into deep saline aquifers. These aquifers, due to their storage capacity and proximity to emission sources, are prime candidates for CO2 sequestration. The near-wellbore environment experiences significant thermo-hydro-mechanical-chemical (THMC) perturbations, necessitating a comprehensive understanding through experimental tests and simulations to maximize the safety and cost-efficiency of CO2 storage. The injection of large volumes (on a million-ton scale) of supercritical CO2 into the geological formations causes evaporation of formation water near wellbores and precipitation of salt crystals inside the porous medium. CO2-induced salt precipitation can substantially threaten sequestration in saline aquifers. While existing works primarily focus on predicting salt location and amounts, our study delves into the physics, growth dynamics, and behavior of the fluid-solid interface near the evaporation/precipitation front. We present a series of experiments, including microfluidic, hele-shaw, and sandbox, along with pore-scale reactive transport modeling using the Lattice Boltzmann Method (LBM), providing fresh insights into brine evaporation and salt growth dynamics. Our research challenges the current understanding, revealing a common shortcoming in many experimental studies—failure to facilitate access and replicate in-situ continuous brine sources. This shortcoming significantly alters the dynamics of salt nucleation and growth in porous reservoir rocks, where the availability and continuity of solute through water film movement control geometric alterations. To address this issue, we also designed surface mineral precipitation tests and large-scale sandbox experiments to investigate salt precipitation and growth under two scales and regimes in porous geometries. The laboratory results indicated massive salt accumulation close to the injection port and underlined the effect of solute availability and continuity on the intensifying severity of salt accumulation. The research outcome highlights the interplay of complex processes (some of which are not yet fully characterized) crucial in investigating salt precipitation induced by million-tons-scale CO2 injection. The observed characteristics call for further in-depth investigation because, in the context of subsurface CO2 storage, we need to redefine how we see injectivity impairment due to salt precipitation.

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MS06-A / 300

Pattern transition during immiscible displacement of non-Newtonian fluids in a rough fracture

Author: Zhibing Yang[1]

Co-authors: Le Zhang [1]; Yves Méheust [2]; Insa Neuweiler [3]; Ran Hu [1]; Yi-Feng Chen [1]

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Two-phase flow in fractured media involving non-Newtonian fluids is of vital importance in many subsurface engineering applications. However, the impact of non-Newtonian rheology on the displacement dynamics remains unclear. In this work, we perform primary drainage experiments in which a Xanthan gum solution displaces a silicone oil in a transparent rough fracture for a wide range of shear-thinning property (controlled by polymer concentration) and flow rates. Based on qualitative and quantitative analyses of the observed fluid morphologies, we present an experimental phase diagram of the obtained displacement patterns. We present an experimental phase diagram of the obtained displacement patterns. We characterize a novel displacement pattern where the fluid-fluid interface changes from stable (plug flow) to unstable (fingering). We further propose a theoretical model elucidating the mechanisms behind the flow regime transitions. The interface stability criterion predicted by this model is in good agreement with the experimental measurements, and stresses the important role of fluid rheology, coupled to aperture variability, in immiscible displacements in rough fractures.

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MS04 / 301

Pore-scale network modelling of CO2–shale interaction with swelling effect

Author: Amin Taghavinejad[1]

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Underground CO2 storage is a crucial effort to reach net-zero carbon emissions by 2050. By this, a large volume of gaseous CO2 is stored underground. Shale formations due to their proper storage capacity—composed of both bulk and adsorption types—can host CO2 for geo-sequestrations. Shale is also a common lithology of cap rocks over underground storage sites, which has the duty of sealing the storage site impeding upward migration of injected CO2. To understand dynamic behaviour of CO2 storage in shales, pore-scale insights are required to investigate physiochemical interactions between injected CO2 and host shale rock. Shale swelling defined as shale matrix deformation due to CO2 adsorption leading to fracture size change is to be studied in this research. In this study, we take an image-based approach to extract unstructured triple-porosity pore-network models (PNMs) based on volumetric synthetic images. At nanoscale, meso- and micro-pores of shale matrix together with fractures compose a network of pores for each shale sample. Various flow features of shale including gas rarefaction, sorption, and surface diffusion are included. It should be noted that this PNM benefits from considering gas sorption effect at pore-level, which is less included in previous shale PNM studies.

By considering methane (CH4) as the host fluid within the pore network and considering injection of carbon dioxide (CO2) into shale samples, effect of swelling is studied. Such that, matrix deformation due to gas sorption imposes a size-reducing effect on fractures. This swelling effect is in competition with mechanical effective stress effect by which fractures are prone to size change as well. Thus, this study computes dynamic pore-scale fracture size change during the injection of CO2 into initially CH4-bearing shale samples. The results give insights into the fracture permeability change in two sets of low-density and high-density fractured shale samples. The results show how Darcy and Knudsen permeability values change over different CO2 injection pressures for both low-density and high-density fractured samples.

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Poster / 302

How does surface salt crystallization influence saline water evaporation from porous media in the presence of a water table?

Author: Sahar Jannesarahmadi[1]

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Saline water evaporation from soil is ubiquitous in many environmental and hydrological processes such as soil water evaporation, vegetation and crop production. It plays an important role on soil salinity influencing soil health and ecosystem functioning. When the salt concentration in soil substantially exceeds its solubility limit as a result of water evaporation, salt crystallization occurs (1). Although how different parameters such as type of salt, soil texture, angularity of the grains, presence of a water table and atmospheric condition influence the formation (1-6), patterns and dynamics of crystallization is relatively well understood, how exactly the presence of crystalized salt influence the evaporation dynamics is poorly understood with the majority of the previous investigations offering qualitative description. We thus aimed at quantifying the effect of crystallized salt on dynamics of saline water evaporation from porous media under controlled laboratory conditions. To do so, three sets of experiments were conducted using NaCl solutions of 10%, 15%, and 20% (mass basis) in a climate chamber with constant air temperature and relative humidity of 30 ℃ and 30%, respectively. Sandy soil with particle sizes ranging from 0.4 to 0.8 mm and density of 2.65 gr/cm3 was used as the model porous medium packed in cylindrical glass columns (20 cm height - 8 cm diameter). The columns were supplied from Marriott's flasks to keep the columns fully saturated during the evaporation experiments. Mass loss from sand samples was measured digitally while crystallization dynamics and their corresponding thermal signatures were monitored with a high resolution optical camera and a thermal imager, respectively. This setup enables us to quantify the contribution of crystalized salt on evaporation. Our preliminary results highlight the key role of salt crystallization on changing evaporation dynamics from sand columns relative to the reference sample supplied with freshwater. Despite the impact of salinity in reducing saturated vapor pressure, we observed enhanced evaporation rates from samples with crystalized salt at the surface by a factor of 4 to 12 (depending on the salt concentration). Furthermore, highly resolved surface temperature dynamics recorded by the thermal camera enabled us to investigate the correlations between the intermittent temperature fluctuations of salt crystals and the evaporative flux from the surface. Our findings provide new insights regarding how the presence of crystalized salt at the surface influences the soil evaporation dynamics.

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MS01 / **303**

Water Thin Films on Kaolinite Gibbsite and Edge Surfaces and Their Effects on Surface Wettability in Relation to Geological Carbon Sequestration

Author: Zhehui Jin[1]

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Geological carbon sequestration (GCS) in subsurface media is one of promising approaches to alleviate excessive CO2 emission 1, while saline aquifers are ideal GCS sites [2, 3]. Generally, four trapping mechanisms including: structural/stratigraphic trapping, residual trapping, solubility trapping and mineral trapping are proposed for GCS in saline aquifers [4, 5]. Among them, structural trapping plays a dominant role in the early stage of GCS, during which CO2 can be sealed in porous media thanks to the capillary pressure between CO2 phase and water phase [6, 7], which is dependent on CO2-water-rock contact angle. It is reported that clay minerals such as kaolinite, account for a large proportion in caprocks. Thus, the knowledge about CO2-water-kaolinite contact angle is of great importance for CO2 structural trapping.

Kaolinite is a typical 1:1 type clay, consisting of one tetrahedral sheet and one octahedral sheet, which are known as siloxane and gibbsite surfaces, respectively [8]. Previous experimental and computer simulation studies [9-12] have shown that kaolinite gibbsite surface is hydrophilic, while siloxane surface is moderately hydrophobic [12]. Although these studies offer general understanding about CO2-water-kaolinite contact angle, they have notable limitations. For example, it is extremely challenging to distinguish kaolinite surfaces in experiments, while the kaolinite surfaces used in experiments are often coated with quartz [11] and soil [9], and sample qualities are highly dependent on their preparation processes [13].

While CO2-water-kaolinite contact angle on two kaolinite basal (gibbsite and siloxane) surfaces has been heavily studied [14], the contact angle on kaolinite edge surface remains unclear. Bickmore et al. [15] reported that the ratio of kaolinite edge surface area to total surface area can be up to ~50%. The water-edge surface interactions, interfacial water structures, and edge surface wettability still remain unknown. Kaolinite edge surface is not atomically flat [16, 17], while surface wettability is also dependent on surface roughness [18]. To the best of our knowledge, kaolinite edge surface wettability in CO2-water-kaolinite system has not been reported yet.

Thus, in this work, we use molecular dynamics simulations to investigate kaolinite gibbsite and edge surfaces wettability in CO2-water-kaolinite systems and elucidate the effect of interfacial water structures at a typical GCS condition (330 K and 200 bar). We find that both gibbsite and edge surfaces are strongly water-wet, while CO2-water-kaolinite contact angle (i.e., 180°) on edge surface is even larger than that of gibbsite surface (i.e., 153°). Due to strong surface atomistic heterogeneity, water thin films with muti-layered hydration structures emerge on edge surface by forming complex hydrogen bonding networks and deplete CO2 molecules from the surface. On the other hand, in the presence of CO2 molecules, water thin films on gibbsite surface consist of single water adsorption layer.

Collectively, our work provides important insights into the dependence of water thin films and interfacial water structures on surface heterogeneity and their effects on surface wettability in CO2-water-kaolinite systems, enhancing fundamental understanding about CO2 structural trapping for GCS.

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MS20 / 305

Preliminary results for a novel in vitro MRI-based approach to quantify blood clot permeability

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Blood clots are a complex heterogeneous porous matrix primarily composed of platelets, red blood cells, and fibrin. This matrix composed of micron and sub-micron scale components results in pores on the order of microns, which causes high flow resistance through the clot in occluded vessels 1. Elevated flow resistance in these occluded vessels, as occurs in cases of stroke or heart attack, results in poor blood perfusion, reduces fibrinolytic protein transport to the clot, and limits the clot lysis rate during thrombolytic therapy. Quantifying blood clot permeability in both statically and dynamically formed clots, which may vary significantly [2], is critical to understanding thrombolytic efficacy and vessel reperfusion. Although previous studies have quantified permeability [2,3], a thorough understanding of blood movement through the porous clot structure remains elusive. This study aims to quantify blood clot permeability using two methods: an established method and a novel MRI-based method.

The first method followed the benchtop permeability experiments detailed by Wufsus et al. [3]. Briefly, a test chamber was occluded with clots of reconstituted platelet rich plasma formed over 24 hours. A saline solution reservoir was attached to the test chamber, and fluid was allowed to permeate through. Flow rate was calculated using a camera to track fluid velocity in tubing downstream of the clot. Permeability was calculated using the Darcy equation and the known fluid viscosity, flow rate, and pressure gradient across the clot. The second method used magnetic resonance imaging (MRI) to track fluid permeation (Fig. 1A). The occluded test chamber was attached to a saline solution reservoir with MRI contrast agent Gadavist® (Bayer HealthCare) at a 1000:1 dilution and placed inside a 14 Tesla MRI scanner (Bruker). Three-dimensional scans of the test chamber were taken using a FLASH pulse sequence with echo and repetition times of 3 and 30 ms, respectively, resulting in a 100 x 100 x 200 microns squared voxel resolution and 3.5 minute scan time. This scan time was sufficiently low to prevent significant signal loss due to fluid motion. Sequential scans were taken over the course of an hour. Avizo was used to generate volumetric reconstructions of the high-intensity fluid domain and calculate flow rate (Fig. 1B).

Results from both methods produced similar average permeability measurements. The average permeabilities from the camera tracking and MRI methods were 5.87E-2 microns squared and 3.86E-2 microns squared, respectively. Although average results were similar, variability between clots were relatively high. These permeability values were slightly higher in magnitude compared to previously reported results by Wufsus et al. for platelet rich plasma clots with low platelet volume fractions (1.2E-2 +/- 0.6E-2 microns squared) [3]. The MRI method had the added benefit of tracking the entire fluid volume through the clot to observe any significant permeation heterogeneities. The fluid moved uniformly through the clot across the entire cross-sectional area, which indicates in this fully occlusive state where fluid motion is primarily governed by Stokes flow, a homogeneous porous media modeling approach may still be appropriate in macroscopic-scale modeling.

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Poster / 306

Pore-scale analysis of fluid transport in different grades of brain tumours considering the effect of extracellular matrix

Authors: Yi Yang[1]; Tian Yuan[2]; Rui Li[1]; Yingfang Zhou[1]; Dubravka Pokrajac[1]; Wenbo Zhan[1]

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Glioblastoma (GBM), one of the most common aggressive brain tumours, accounts for more than 50% of primary malignant central nervous system (CNS) gliomas in adults. According to the World Health Organization (WHO) classification 1, brain tumours can be graded from 1 to 4 as pilocytic astrocytoma (PA), diffuse astrocytoma (DA), anaplastic astrocytoma (AA) and GBM in terms of malignancy and abnormality. GBM remains challenging to treat with a high 5-year modality rate of more than 90%. This undesirable efficacy can be partially attributed to the higher levels of the extracellular matrix (ECM), thereby leading to disappointing drug delivery outcomes. Hyaluronic acid (HA), one of the major components of ECM, is 8 times and even higher in GBM than the HA level in brain normal tissue, However, how HA affects the ISF transport in the microscale channels is insufficiently understood.

In this study, we first reconstructed the different 3D tumour microstructures from Grade 1 to 4 based on the microscopic morphology of U87 cell lines and their geometrical information (porosity and cell size) [2]. We conducted the simulations using the open-source computational fluid dynamics software OpenFOAM [3]. We confirmed the representative element volume (REV) size (200 μm) and validated simulation results with the reported experimental results [4]. We then quantified the relationship between tissue hydraulic permeability and HA concentration in the low- and high-grade tumours. Specifically, we indicated that the average permeability between PA and DA decreases by 23.5% with an average 21.6% increase of porosity and the same level of HA deposition. While the average porosity increased by 33% from the low-grade to the high-grade tumours, the mean hydraulic permeability decreased by 23.8% with the 2.7 times increase in the HA concentration range. We identified the necrotic region (NR) in GBM as more permeable than high-grade tumours, due to the highest porosity and relatively lower HA concentrations. Therefore, results from our computational models underscore the dominant effect of the HA matrix when simulating the ISF flow in brain tumours. Finally, we established a significant correlation between hydraulic permeability and HA concentration range in different grades of brain tumours, and also found that low- and high-grade tumour tissues are more permeable than brain normal tissues [5].

In this work, we developed a modelling framework to investigate the ISF transport in different WHO Grades of brain tumours. We also linked the ECM permeability to ISF flow through the extracellular space on the pore scale. The findings from this work can advance the accuracy of prediction of fluid transport properties in the brain tumour, and hence also the efficiency of potential drug delivery strategies for brain tumours and other disorders.

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MS20 / **307**

Investigating charged nanoparticles diffusion in brain tumour microstructures at pore-scale

Authors: Yi Yang[1]; Tian Yuan[2]; Rui Li[1]; Dubravka Pokrajac[1]; Yingfang Zhou[1]; Wenbo Zhan[1]

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Nanoparticles (NPs) have emerged as promising candidates for targeted drug delivery in the treatment of brain tumours due to their diverse physicochemical properties. With the advanced development of convection-enhanced delivery (CED), anticancer drugs are directly infused into the targeted brain tumour region through a catheter, enabling drugs to bypass the blood-brain barrier (BBB). Multiple factors, such as particle size and surface charge are crucial for enhancing the NP transport in brain tumours 1. However, primarily owing to the complex microstructure and microenvironment of the brain tumours, how these physical properties affect the NPs diffusion in the brain tumour at pore-scale still needs to be clarified and quantified.

In this study, we first established a framework consisting of different geometrical models of brain tumour microstructures from Grades 1-4 [2] and the particle tracing model to investigate the relation between the effective NP diffusion coefficient in brain tumours and their physical properties. We verified the predictive power of the present model by comparing the results under the same conditions to experimental results reported in the literature 1. Then, we quantitatively analysed the NP diffusion coefficient in order to establish the effect of particle size, surface charge, temperature and extracellular matrix. We found that the diffusion coefficients of NPs are positively related to all these physical properties when the total surface charge increases with the particle size [3]. Conversely, the diffusion coefficient of NPs negatively corresponds to the particle size when the total surface charge is kept the same. The magnitude of the diffusion coefficient with the zeta potential (Zp) of -5mV is at least 1500 times larger than that value of uncharged NPs. This difference is even more pronounced with larger NP sizes. More interestingly, we noted that the diffusion coefficient in the high-grade tumour microstructures is smaller than that in low-grade tumour microstructures when other parameters are kept the same, although the high-grade tumours possess a higher porosity than low-grade tumours. This may imply that higher level of hyaluronic acid (HA) of ECM deposited within the interstitial fluid is essential for the critically decreased diffusion coefficient in high-grade tumours.

Results from this study can deepen the understanding of the relationships between NP diffusion coefficient and physical characteristics of NPs in brain tumours, providing crucial insights and a reliable modelling framework for the development of nano-drugs and carrier delivery processes in chemotherapy of brain tumours and other brain disorders.

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MS13 / 309

Wetting behaviors and oil occurrence status of shale reservoirs

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A contrast-variation technique in small-angle neutron scattering (CV-SANS) is employed to investigate the interfacial chemistry of shale oil reservoirs using reagents that span a range of polarities, including water, toluene, and dimethyl methanamide. Through five different experimental strategies, the work demonstrates a modification of shale wettability, ranging from enhancement, weakening, to reversal. This study also presents an innovative approach for characterizing the status of oil occurrence at the nanometer scale, and new insights into the scattering vector-particle size (q-r) relationship in polydisperse systems. The unique CV-SANS technique shows that shale with low contents of total organic carbon, clays, and porosity typically indicates better oil mobility, associated with larger particle scales. Meanwhile, the results indicate that an increase in pore scale does not necessarily accompany the rise in radius of gyration when mass density spatial variation occurs in the system. Collectively, this work establishes a direct correlation between size r in real space and q in reciprocal space and decodes the interfacial wettability traits in nanopores of shale oil reservoirs.

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Poster / 310

The occurrence states of shale oil and its controlling factors in Yanchang Formation, Ordos Basin, China

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Oil mobility evaluation is the primary topic in shale oil development. The different occurrence states of shale oil, which closely relate to the pore structure and fluid properties tremendously affect the oil mobility in shale. As proved in previous studies, the higher the content of oil in free states, the better the oil mobility will be. In this study, the oil occurrence states and its influencing factors of the 7th member in Yanchang Formation (Chang7) in Ordos Basin, China were investigated by multiple experiments, including nuclear magnetic resonance (NMR), nitrogen gas adsorption (NGA), electronic scanning microscope (SEM), X-ray diffraction, and rock pyrolysis. The Chang7 samples were classified into four lithofacies based on mineralogy and TOC. With the increasing of the clay content, the four lithofacies are siliceous shale, OM-rich siliceous shale (TOC>5%), argillaceous shale, and OM-rich argillaceous shale (TOC>5%) (Figure 1). The NMR results indicate the fluids in Chang7 consist of structure water, free water, adsorbed oil, and free oil. The contents of adsorbed oil increase with TOC and clay percentages increase. However, the contents of free oil show negative relationships with TOC and clay percentages. Therefore, we speculate that the strong adsorbability in organic matter and clay minerals force the oil to be preserved as adsorbed oil in shale, which tremendously affect the oil occurrence states and mobility. Siliceous shale has the greatest content of free oil, and OM-rich siliceous shale has the greatest content of adsorbed oil. From the NGA results, mesopores have the domination in pore volume and specific surface area, especially in siliceous shale. The cumulative pore volumes decrease from siliceous shale to OM-rich argillaceous shale with the increase of clay contents. The NGA was also conducted on the samples after solvent extraction, which shows opposite changes of the volume in mesopores and macropores. Lots of mesopores were released by solvent extraction, particularly in siliceous shale which has the greatest increase in mesopores. Similarly, SEM images of the siliceous shale also show a large amount of mesopores in felsic grains. In the other three lithofacies, few pores were observed because of the tight compaction of clay and felsic minerals. Combing with the free oil content, the positive relationship between the free oil content and different percentage of mesopore volume indicates that the mesopores are the primary storage space of free oil (Figure 2). Compared with the lithofacies which have more clay content and TOC, the siliceous shale has more mesopores and low adsorbability in the pore system, which provides an optimum pore structure for the occurrence of free oil. To summarize, the free oil content shows an obvious preference in siliceous shale. The lithofacies defined by mineralogy compositions and TOC affect the oil occurrence states by pore structure. Parallelly, the pore structure was deeply affected by the grain size, spacial arrangement, and minerals (grain type). Therefore, the occurrence states of oil in shale were strongly affected by the pore structure through the lithofacies.

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Poster / 311

Mechanism simulation on low salinity water flooding in high temperature sandstone reservoirs based on molecular simulation method

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Low salinity water flooding (LSWF) is novel technique which can be used to improve oil recovery for sandstone reservoirs. Although considerable experimental research has been conducted to identify the underlying pathways, there are a lot of debatable issues with the mechanics. On the basis of molecular simulation (MS) method, the models of rock, oil and brine in different salinity and ions compositions were constructed. The interactions among rock, oil and brine and the influence of brine salinity and concentrations of ions on the process of separating oil from sandstone surfaces were studied. The temperature range considered ranged from 298K to 373K. That altering of the wetting state of a sandstone induced the detachment of oil from the surface of the rock, even under elevated temperatures. The results will provide essential molecular state information for change in the wetting state of rock and increase in oil recovery.

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MS09 / 312

Multiphase Reactive Transport Modeling of CO2 Dissolution in Geological Carbon Sequestration Using Lattice Boltzmann Simulations

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Geological carbon sequestration is the most suitable way to alleviate the negative influence caused by CO2 at the field scale. CO2 dissolution as one of the most indispensable and predominant trapping mechanisms is a complicated process involving both physical and chemical phenomena. In this work, CO2 dissolution after capillary trapping far away from the injection well under different environmental conditions is investigated to elaborate the main controlling mechanisms of CO2 dissolution reactions and the corresponding sensitivity analysis during these processes.

Coupled with homogeneous reactions in the brine and heterogeneous reactions at the CO2-brine interface, a multiphase Shan-Chen multiple-relaxation-time lattice Boltzmann model with multicomponent transport is established to capture CO2 dissolution reactions with phase transitions in saline aquifers. Controlling mechanisms of CO2 dissolution reactions are probed by estimating the temporal evolution of CO2(aq) concentration and the dissolved CO2 nodes under different diffusion coefficients and CO2 saturations in a periodic domain. Furthermore, CO2 dissolution in porous media is captured to explain the ion evolution during homogeneous reactions and characterize the impact of different factors, namely partial pressure, formation temperature and salinity, on this process in the view of practical application.

The rapid mass transport, namely the large diffusion coefficient, could keep the CO2(aq) concentration gradient at the scCO2-water interface at a high level, which would accelerate CO2 dissolution processes. The ratio of the equilibrium time between various cases is nearly about 3 times. Additionally, the reactive interfacial length also affects CO2 dissolution reactions. It can be concluded from the simulated results that higher reactive interfacial length would make the security of CO2 trapping greater under the same CO2 saturation. More importantly, it is found that the CO2 dissolution process is non-equilibrium and would not be omitted when the sequestration efficiency is estimated in reservoir-scale simulations. Otherwise, the accuracy of the results cannot be ensured. It is beneficial for sequestration efficiency to adopt the high-pressure region due to greater CO2 density and equilibrium concentration at the scCO2-water interface. Besides, the formation temperature, which should be prudently selected in the targeted saline aquifer for practical operation, has both positive and negative effects on CO2 dissolution. In terms of salinity, the more ion strength is the less trapping efficiency is.

This study offers not only a deeper understanding of multiphase reactive transport of CO2 dissolution in porous media during geological carbon sequestration but also a new idea about the same physicochemical backgrounds, such as the hydrogenation of levulinic acid.

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MS15 / **313**

Multiparameter Inversion of Reservoirs Based on Deep Learning

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Reservoir parameter inversion is an important technique in oil and gas exploration and development that can estimate the reservoir physical properties, such as skin factor and permeability, using observed data, such as well test data and production data. In this paper, we propose a physical accelerated neural network with multiple residual blocks (PRNN-Acc) for multiple parameter inversion of the seepage equation with a source term and a sink term. PRNN-Acc is based on the idea of physical residual neural network (PRNN), which uses deep neural networks to approximate the solution and parameter spaces of partial differential equations. PRNN-Acc adds multiple residual blocks to enhance the expression ability and flexibility of the network and avoid gradient explosion or degeneration phenomena. In addition, the input of PRNN-Acc is multiplied by three adaptive parameters, which can adjust the network training process according to the characteristics of the data and loss function and improve the accuracy and stability of the inversion. We use bottomhole pressure (BHP) data before and after shut-in as labels to invert multiple parameters for homogeneous and heterogeneous reservoirs. In this paper, three numerical experiments are designed. For homogeneous and heterogeneous reservoirs, the inversion results of this method are up to 36 times more accurate than those of PRNN. It is fully proven that the inversion effect of this method is better than that of PRNN.

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MS06-A / **314**

A microfluidics investigation of the impact of microfractures on flow patterns in porous media during imbibition

Authors: Bowen Zhang[None]; Zhonghao Sun[1]

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The imbibition in porous media plays a critical role in various natural and engineering processes, such as rainfall infiltration, hydrocarbon recovery, geological CO2 storage, and environmental remediation. Microfractures and discontinuities are naturally presented and purposely induced in natural rocks and soils. The interaction between these heterogeneities and the matrix increases the complexity of multiphase flow behavior in porous media.
This study aims to investigate the impact of microfractures on flow patterns in porous media during imbibition and understand the pore-scale fluid interaction between microfracture and matrix via microfluidics experiments. Polydimethylsiloxane (PDMS) micromodels of fracture-matrix porous media with various fracture widths are designed and fabricated using the soft lithography technique. The width of the matrix channels follows a lognormal pore-size distribution with a mean size of 30 and a standard deviation of 0.4. The width of the fracture varies from 4 to 40 times the mean pore size (120 μm to 1200 μm). The depth of the channel is around 110 μm. We inject ethanol as the wetting phase to displace air at various flow conditions (constant flow and constant pressure). A pressure transducer at the inlet monitors the pressure change, and a fluorescent microscope records the flow behavior. The effect of different microfracture geometries on flow patterns during imbibition at various flow conditions is analyzed.
Results show that the flow pattern is matrix-prefer when the injection flow rate is low. The ethanol prefers to invade the matrix, and the fracture acts as a capillary barrier. The flow pattern transfers from matrix-prefer to the transitional stage as the flow rate increases. The liquid equally invades the matrix and fracture area. The interaction between fracture flow and matrix flow is observed. Eventually, the fracture becomes a preferential channel at high flow rates. The capillary barrier and preferential channel phenomena are less salient for narrow fractured porous media, whereas they become more significant as the width of the fracture increases. The recorded pressure signatures reveal that the interplay between capillary and viscous forces results in different flow patterns during imbibition. The capillary force dominates the flow behavior at low capillary numbers and imbibes the wetting phase into the matrix. Fractures act as capillary barriers when the fluid pressure is smaller than the entry pressure. The viscous force dominates the flow behavior as the capillary number increases. The wetting phase invades the low-viscous drag fracture and the cross flow between fracture and matrix is limited.
In conclusion, we observe three flow patterns in fractured porous media during imbibition and identify two thresholds for these patterns. The interaction between fracture flow and matrix flow is analyzed at the pore-scale, Results presented in this study are relevant to the understanding of multiphase flow phenomena in fracture-matrix systems at various flow conditions.

Keywords: Microfracture, heterogeneity, imbibition, microfluidics, flow pattern, porous media

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Poster / 315

Attenuation Patterns of Low-Frequency Hydraulic Pulse Waves in Porous Media with Different Permeability

Authors: Kai Wang[1]; Qiao Fan[1]; Yunzhi Ge[1]; Yuanjia Lv[1]; Yuchi LI[1]

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Hydraulic pulsing is a widely used technology for cleaning, hydro-shredding, and soil improvement. In recent years, low-frequency hydraulic pulses have been used in oil and gas development, such as wellbore blockage removal and EOR. The effectiveness of this process depends on the attenuation pattern of the hydraulic pulse wave in the reservoir. In this paper, a numerical model of low-frequency hydrodynamic pulsed wave propagation in porous media is constructed and experimentally verified. The finite element method was used to solve the model and analyze the radial attenuation patterns of low-frequency hydraulic pulse waves in porous media with varying permeability. The results indicate that the rate of attenuation of the energy (pulse amplitude) of the hydraulic pulse wave with distance is significantly affected by the permeability of the porous medium. The rate of attenuation exhibits a pattern of deceleration, acceleration, and then deceleration again as distance increases. As the hydraulic pulse frequency is 0.1Hz, the pulse amplitude is 10MPa, and, the pulse amplitude attenuates faster along the path as the permeability decreases and is mainly concentrated within 0.5-2.5m around the wellbore. Specifically, the pulse amplitude attenuation to 20% corresponds to a propagation distance of 1.8 m in the 1 mD porous media, 2.7 m in the 200 mD porous media, and 6.8 m in the 1000 mD porous media. The pulse amplitude gradually decreases within 0.5 meters around the wellbore, which may be attributed to the impact of reflected waves. In a porous medium with a permeability of 100 mD, reducing the pulse frequency (0.1-30 Hz) can effectively decrease the interference between different wave levels during propagation and slow down the attenuation rate of pulse amplitude with distance. As distance increases, the effect of pulsation amplitude on attenuation decreases, and the degree of attenuation becomes similar for different amplitudes. For reservoirs with specific permeability, it is recommended to adjust the hydraulic pulse parameters to a lower frequency and higher amplitude to achieve a longer effective distance and better results.

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MS03 / 316

Research on Fracture Propagation Law of Shale Hydraulic Fracturing Based on Mineral Interface Effect

Author: Mengru Hou[None]

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To address the scientific problems of fracture initiation and expansion of hydraulic fractures in the process of shale gas reservoir extraction, this paper focuses on the influence of shale minerals on fracture initiation and expansion of hydraulic fractures under the influence of mineral interface, establishes a geometric model of random distribution of shale minerals at the microscopic scale, and uses the cohesion model to characterize the mineral interface, and constructs a microstructure model of shale considering the influence of mineral interface. Numerical simulations are used to study the effects of mineral interface stiffness, mineral content and mineral grain size on hydraulic fracture expansion, and the fracture expansion pattern of shale hydraulic fracture under the influence of mineral interface is obtained. The results of the study help to reveal the mechanism of shale minerals on hydraulic fracture extension under the influence of mineral interface, and provide a theoretical basis for the reasonable selection of hydraulic fracturing layer in shale gas reservoir. The results show that.
(1) The mechanical response of mineral interface to shale is more obvious, and when subjected to external force, the damage appears first at the mineral interface, and then the damage starts to occur gradually inside the mineral, and the damage inside the quartz mineral is the largest, and the damage inside the clay mineral is the smallest. (2) As the stiffness of mineral interface increases, short and wide cracks are formed more easily; as the percentage of brittle minerals increases, long and wide cracks are formed more easily; when the mineral grain size increases from 40μm to 60μm, long and wide cracks are formed more easily, and when the mineral grain size increases from 60μm to 80μm, short and narrow cracks are formed more easily, and the form of crack damage is mainly tensile damage. (3) The shale hydraulic fracturing operation should give priority to the fracturing of layers with low mineral interface stiffness, high brittle mineral content and large mineral grain size, which is conducive to the construction of seepage channels in shale reservoirs and improving the transport capacity of shale reservoirs.

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MS17 / 317

Study on pore-fracture morphology and mineral-induced acid-heat-flow-solid simulation of coal under supercritical CO2

Author: Saipeng Huang[1]

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Introduction
Carbon capture and storage (CCS) in geological reservoirs has emerged as a rapidly effective op-

tion for mitigating the accumulation of greenhouse gases [1,2]. However, the flow and reactions of supercritical CO2 (SCCO2) within coal seams entail a complex process, encompassing minerals dissolution and precipitation, adsorption behaviour, microstructural changes and mechanical weakening effects [3]. These factors hold a crucial role in ensuring the secure and long-term geological storage of CO2 in deep reservoirs. However, existing models mainly focus on temperature, flow and mechanics, leaving a significant gap in the multi-physics field considering the effect of SCCO2 acidification on coal structure in deep reservoir. On this basis, a comprehensive acid-thermal-flow-solid model was developed and established to account for mineral dissolution processes. This model was employed to study the influence of coal pore-fracture morphology and mineral distribution on the assessment of SCCO2 geological sequestration in deep reservoirs, thereby addressing the limitations inherent in existing models concerning the characteristics of CO2 storage in deep reservoir.
Methodology
A geometric model representing a circular reservoir was constructed. Within this model, the wellbore radius was defined as 0.1 m, while the radius of the matrix region was established at 1 m. The mesh distribution employed throughout the simulation is depicted in Fig. 1. Natural fracture distributions were incorporated in the model, with the permeability of these natural fractures typically being 1,000 times that of the matrix permeability.
Results and Discussion
A reduction in porosity was observed radiating from the wellbore towards the boundaries under interactions with SCCO2, with this distribution being influenced by fractures. An increase in the initial porosity of the coal samples corresponded to a more significant alteration in porosity after exposure to SCCO2, as depicted in Fig. 2. Following SCCO2 interaction, reservoir porosity increments resulting from adsorption expansion, dissolution, and total porosity were observed to decrease with an increase in initial porosity. The reservoir's total porosity was found to be 1.24 to 1.56 times that of its initial state after SCCO2 treatment. The increase in total reservoir permeability was found to intensify over time; nevertheless, as the reservoir's initial porosity increased, this enhancement was decreases gradually. For coal samples with initial porosities of 0.05, 0.06, 0.07, 0.08, 0.09, and 0.1, the corresponding permeability increments were determined as 23.57, 15.11, 10.45, 7.80, 6.11, and 4.98, respectively. This indicates that the lower the initial porosity of the reservoir, the more pronounced the alteration of its flow characteristics by SCCO2.

Fig. 1. Geometric model and simulation results. a) The grid distribution of the reservoir's geometric model. b) The porosity distribution of reservoirs with different initial porosities after exposure to SCCO2. c) The variation in porosity of reservoirs with different initial porosities after exposure to SCCO2. d) The variation in permeability of reservoirs with different initial porosities after exposure to SCCO2.

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MS04 / 318

Impact of Sand-Hydrogel Mixtures Swelling on Shearing Behaviour: An X-ray CT Study

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Hydrogels also known as superabsorbent polymers (SAPs) are crosslinked hydrophilic polymers characterized by a three-dimensional polymer network structure. These polymers are capable of absorbing water to thousands of times their own weight. Hydrogels can either be synthetic (polyacrylic acid) or natural such as biopolymers (xanthan gum). The use of hydrogels has been found to have increased utilization in diverse fields such as agriculture, environmental science, petroleum, and civil engineering. The key attractions in the use of hydrogels in these fields include the ability to absorb substantial amounts of water, selectively attracting and binding to pollutants and facilitating particle aggregation. Most previous studies have consistently demonstrated that during wetting swelling of hydrogel leads to restructuring of the soil particles and these studies claim that results of wetting affect the soil stiffness, increases erodibility, and reduces shear strength. However, we lack a more comprehensive understanding of the complex micromechanical processes that govern the behaviour of hydrogel-treated soils during wetting. This knowledge gap hinders our understanding of the interaction of hydrogels with soil and the effective use of hydrogels in soil remediation and geotechnical engineering applications. This study aims to unravel the swelling process of hydrogel in soil, how it leads to restructuring of soil particles and the resulting impact on the mechanical behaviour of hydrogel-treated soils. We employ a miniature triaxial cell connected to a humidifier and a peristaltic pump to supply humid air during saturation of the sand-hydrogel mixture. We utilize an X-ray Computed Tomography (CT) scanner to unveil the four-dimensional (3D + time) perspective of swelling-induced disturbance and its impact on the shearing behaviour. Preliminary results show that hydrogel swelling dramatically reduce sand-to-sand contacts, resulting in a much smaller peak strength. We further adopt image processing algorithms to denoise, segment phases (sand, hydrogel, and air), and label sand and hydrogel particles for performing quantitative analysis such as displacement and strain fields.

KEY WORDS: Hydrogels; Swelling; Shearing behaviour; Soil restructuring; X-ray tomography.

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MS15 / 319

Feasibility study of the inversion method for non-uniform hydrate saturation distribution based on ensemble Kalman filter algorithm

Author: Yongge Liu[1]

Co-authors: Xu Zhang [1]; Jian Hou [1]; Guo Li [1]; Hongzhi Xu [2]; Ermeng Zhao [1]; Litao Chen [1]; Tiankui Guo [1]; Evgeny Chuvilin [3]

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Field tests and laboratory experiments indicate that the spatial distribution of hydrate saturation in hydrate reservoirs is non-uniform. This non-uniform distribution significantly impacts the reservoir' s temperature changes, and gas and water production rates during reservoir development. Currently, the primary methods for determining hydrate saturation distribution in porous media are nuclear magnetic resonance (NMR) and computed tomography (CT) scanning. However, these methods have limitations such as small detection ranges, high costs, and the necessity of interrupting experiments. During depressurization exploitation of hydrate reservoirs, abundant data on gas and water production, as well as temperature and pressure monitoring, are available. These highly reliable observational data vary with changes in hydrate saturation distribution, providing the possibility of using inversion methods to determine this distribution.

This study first conducts secondary development of the Tough+Hydrate simulator. Energy and mass conservation equations are separately constructed for the matrix and high-conductivity channels after reservoir stimulation. The transfer of mass and heat in the matrix and high-conductivity channels was characterized using the discrete fracture method. A numerical simulation method for reservoir stimulation assisted depressurization development of hydrate reservoirs was established and implicitly solved. Then, by combining the ensemble Kalman filter algorithm with the simulator, the inversion method of the hydrate saturation distribution was built and then validated using three cases: core scale depressurization development, hydraulic fracturing assisted depressurization development, and radial well stimulation assisted depressurization development. The impact of the number of observation points on the inversion results also was investigated. Finally, based on the observation data of Masuda's classic experiment, the inversion method was used to obtain the distribution of hydrate saturation in the core of Masuda's experiment successfully.

Research results indicate that the established inversion method continuously assimilates observational data in the ensemble. Hydrate saturation distributions obtained through inversion in the three cases tend to approach the preset distributions, demonstrating the reliability of the inversion method. The quantity of observational data has a certain influence on inversion results; more observational data lead to the assimilation of more information, resulting in hydrate saturation distributions closer to the actual values. Inversion results based on Masuda's experimental data reveal a strong non-uniformity in hydrate saturation distribution within the core, with a relatively high hydrate saturation zone in the central region and lower hydrate saturation at the inlet and outlet ends.

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Poster / 320

Investigation on pore structure and imbibition characteristic of tight sandstone by nuclear magnetic resonance

Author: Xuanzhe Xia[1]

Co-author: Jianchao Cai [2]

[1] *China University of Petroleum-Beijing*

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

Corresponding Authors: caijc@cup.edu.cn, xxz1209@163.com

Abstract: Tight sandstone reservoir, as unconventional oil and gas resource with abundant quantity, plays a significant role in supporting the growing global demand of energy consumption. However, tight sandstone has complex pore structure and strong heterogeneity, which brings challenges to the development of unconventional hydrocarbon resource. In recent years, the nuclear magnetic resonance method has been widely applied in porous media with the advantages of nondestructive, fast and wider range of pore size characterization in investigating pore structure. But pore size distribution curve cannot be obtained directly by nuclear magnetic resonance method. The transverse relaxation time spectrum from nuclear magnetic resonance could be converted into the pore size distribution curve by appropriate surface relaxivity, which can be affect by paramagnetic minerals and varies with lithology. Using low temperature nitrogen adsorption method, high-speed centrifugation method, and nuclear magnetic resonance, the surface relaxivity of five tight sandstone samples from different depths of Dongying depression was measured in this study. And then the influence of mineral composition from experimental samples on surface relaxivity was discussed. In addition, the pore size distribution curve from mercury intrusion porosimetry is utilized to verify the accuracy of the pore size distribution curve inversed by the surface relaxivity. Based on the obtained surface relaxivity, imbibition experiments under high temperature and high pressure conditions were conducted combined with nuclear magnetic resonance technique. Then the flow characteristics of whole cores and different pore size types (micropores, mesopores and macropores) influenced by temperature and pressure was analyzed, and the imbibition mechanism of tight sandstones resource was revealed.
Keywords: NMR, Surface relaxivity, Pore size distribution, Imbibition

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MS10 / **322**

Understanding heterogeneous and anisotropic porous media based on geometric properties extracted from three-dimensional images

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Natural porous media is generally heterogeneous and anisotropic. The structure of porous media plays a vital role and is often the source of heterogeneity and anisotropy. In a physical process such as fluid flow in porous media, a small number of major features here referred to as wide channels, are responsible for the majority of the flow. The thickness and orientation of these channels often determine the characteristics of the permeability. Typically, the identification of such major features is conducted through time-consuming and expensive simulations. Here we propose a prompt approach based on geometric properties extracted from three-dimensional (3D) images. The size or radius of the major features is obtained via distance maps, and their orientations are calculated by Principal Component Analysis. We then visualize these features with color and color brightness according to their orientation and size, together with their location and distribution in 3D space, and the simultaneous visualization of anisotropy (orientation) and heterogeneity (size) in one plot provides a straightforward way to enhance our understanding. Furthermore, we propose a refined stereographic projection to statistically illustrate heterogeneity and anisotropy. Based on this understanding, we show a new way to compress model size in numerical simulation, therefore significantly reducing computational cost, while retaining its essential characteristics.

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Poster / **323**

Changes in the acoustic signature of tight sandstone during spontaneous imbibition process

Author: Fangzhou Zhao[1]

Co-author: Jianchao Cai [1]

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Abstract: Spontaneous imbibition is a process in which porous media spontaneously inhales wetting liquid driven by capillary force, which is an effective means to enhance oil recovery in tight reservoirs. At present, the observation methods of spontaneous imbibition mainly include nuclear magnetic resonance method and computer tomography method. In this paper, the method of ultrasonic testing is used to link the change of seismic attributes of rocks with the distribution of fluids, indirectly observe the spontaneous imbibition process of rocks, and explore the imbibition law of tight sandstone. The high-pressure mercury intrusion method and low-temperature nitrogen adsorption method were carried out on two kinds of tight sandstone. The pore structure parameters of the rock were calculated, and the complexity of the pore structure was quantitatively described according to the fractal characterization method. In addition, the ultrasonic test of the imbibition process of the two rocks was carried out, and the flow of the fluid was observed by the change of the velocity and amplitude of the elastic wave, and the influence of the pore structure of the rock on the imbibition was analyzed. The results show that the pore structure of tight core is complex, mainly micron pores. The initial rate of imbibition is faster, and the rate gradually slows down with the increase of imbibition height. When the fluid front reaches the vicinity of the sensor, the velocity and amplitude of the ultrasonic wave are strongly affected.

Keywords: Tight sandstone, spontaneous imbibition, ultrasonic monitoring

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MS06-A / 324

A generic model for capillary imbibition in a liquid-liquid system: Non-Newtonian fluid as the wetting phase

Authors: Pengyu Fu[1]; Yuhang Wang[1]; Huirong Guo[1]; Wanjun Lu[1]

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Capillary imbibition is a widespread phenomenon in both natural and industrial fields. While most studies focused on the imbibition between two Newtonian fluids or the fluid pair composed of a non-Newtonian liquid and air, the imbibition of a liquid-liquid system, where the wetting phase is a non-Newtonian fluid, remains relatively unexplored. Understanding the dynamics of flow for such fluid system is essential in petroleum engineering and the remediation of contaminated aquifers, as the flushing agent is often characterized as non-Newtonian. In this work, we proposed a generic mathematical model to describe the capillary imbibition of a system in which the non-Newtonian fluid acts as the wetting phase. Specifically, we derived the viscous force exerted on the non-Newtonian fluid based on the wall shear rate of Newtonian fluid. The resulting governing equation is applicable to various rheological models of non-Newtonian fluids. The Carruea-Yasuda model is adopted in this work, as it is able to describe the apparent viscosity over a wide range of shear rates. To verify the developed model, we conducted the capillary rise experiment in straight circular tubes, and compared the numerical solutions against physical observations. Two fluid pairs were examined: (1) liquid-air, and (2) liquid-liquid. In both cases, the wetting phase is non-Newtonian. Results show that the good agreement is obtained between the predictions from the developed model and experimental data across all investigated cases. In contrast, the traditional model falls short of capturing equilibrium rise height in the liquid-liquid case. We found that for a liquid-liquid system, incorporating appropriate viscous force into the governing equation is crucial for accurately describing the dynamics of capillary imbibition.

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Multiscale Multifractal Characterization of Pore Fractures in Oil Shale under Temperature Effects

Authors: Dingwei SUN[1]; Dong YANG[1]

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The investigation of the spatial distribution of microscale pores and fractures in oil shale plays a pivotal role in revealing the internal reservoir properties and fluid transport characteristics within the oil shale. The impact of temperature on the generation of internal pores and fractures in oil shale is substantial, and the appropriate temperature and pyrolysis time bear significant importance for the rational exploitation of oil shale. To explore the multifractal characteristics of oil shale pore structures at different scales and their evolution under temperature influence, multifractal characterization was conducted on oil shale samples post-pyrolysis at both micrometer and nanometer scales. Utilizing CT image processing software, the reconstruction of oil shale specimens subjected to pyrolysis at various temperatures was performed. At the micrometer scale, the analysis revealed the

distribution and volume percentages of oil shale pore sizes. Additionally, employing higher precision physical experiments such as mercury intrusion porosimetry, nitrogen adsorption, and carbon dioxide adsorption provided insights into the nanometer-level pore distribution characteristics of oil shale specimens. Fractal methods employed included generalized dimension spectra and multifractal singularity spectra. The results indicate that the pore structure of oil shale after temperature exposure exhibits multifractal characteristics. There is a strong correlation with the magnitude of temperature and pyrolysis time, where temperature exposure promotes homogeneity in the oil shale pore structure and enhances pore connectivity. Furthermore, the spatial distribution of nanoscale pores becomes more intricate.

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MS13 / **327**

Modelling the Effect of Porewall Heterogeneity on the Phase Equilibria of Fluids in Shale Nanopores

Authors: Xiaohu Dong[1]; Zhan Xiao[1]

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Fluid phase behavior in shale nanopores has become a hot topic in recent years. But, most of the current investigations are based on a smooth porewall assumption. Actually, for such small-scale pores in shale, a serious porewall heterogeneity has been observed, which has been confirmed in many experimental observations.
In this paper, the methods of N2 adsorption and desorption measurement, scanning electron microscope (SEM) and atomic force microscope (AFM) are first applied to characterize the pore structure of shale rocks, and three porewall heterogeneity modes are proposed, including furrowed surface, ravine surface and sinusoidal surface. Simultaneously, the corresponding modelling procedure is developed. Then, through a comparison between the experimental observation and simulation results, the optimal porewall heterogeneity assumption is derived. Thereafter, based on a pore size depended equation of state (EOS), with the consideration of capillary pressure, adsorption layer and fluid-solid interaction, a mathematical model for the fluid phase transition behavior in shale heterogeneous nanopores is established. And the porewall heterogeneity on the fluid phase behavior is discussed.
Results indicate that among the three modes, a sinusoidal porewall assumption is the most recommended one with an average relative error (<2%). Our developed mathematical model can well simulate the fluid phase transition behavior in shale nanopores. Compared with a smooth porewall assumption, a consideration of the porewall heterogeneity can further reduce the bubble point pressure. For pure hydrocarbons, with the pore size reduces and molecule weight increases, the effect of porewall heterogeneity is enhanced. For mixtures, with the fraction of heavy component increases, the deviation between with and without the consideration of porewall heterogeneity is increased.

This paper firstly simulates the effect of porewall heterogeneity on the fluid phase behavior in shale nanopores. It sheds some new insights to understanding the phase equilibria of hydrocarbons in shale play.

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MS09 / 329

A thermodynamically consistent and conservative diffuse-interface model for two-phase flows in complex geometries

Authors: Chengjie Zhan[1]; Xi Liu[1]; Zhenhua Chai[1]

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In this work, a thermodynamically consistent and conservative diffuse-interface model for gas-liquid-solid multiphase flows is proposed. In this model, a novel free energy for the gas-liquid-solid multiphase flows is established according to a ternary phase-field model, and it not only contains the standard bulk and interface free energies for two-phase flows, but also includes some additional terms to reflect the penalty in the solid phase and the wettability on the solid surface. Furthermore, a smooth indicator function of the solid phase is also introduced in the consistent Navier-Stokes equations to achieve a high viscosity in the solid phase and preserve the velocity boundary conditions on the solid surface. Based on the proposed diffuse-interface model, the fluid interface dynamics, the fluid-structure interaction, and the wetting property of the solid surface can be described simply and efficiently. Additionally, the total energy is also proved to be dissipative for the two-phase flows in the stationary geometries. To test the present diffuse-interface model, we develop a consistent and conservative lattice Boltzmann method and conduct some simulations. The numerical results also confirm the energy dissipation and good capability of the proposed diffuse-interface model in the study of two-phase flows in complex geometries.

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Poster / 330

Study on Injection-Production Characteristics of CO2 Flooding in Fractured Extra/Ultra-low Permeability Reservoirs

Authors: Xinliang Chen[1]; Hongwei Yu[2]; Zhengming Yang[2]; Ming Gao[2]; Zhongkun Niu[1]; Yilin Chang[1]; Meng Du[1]; Pengwei Fang[1]; Zhuoying Dou[1]; Yuan Gao[1]

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Abstract: Clarifying the injection-production characteristics during CO2 flooding in fractured extra/ultra-low permeability oil reservoirs is significant for further improving oil recovery. This study focuses on the fluid and reservoir characteristics of ultra/low-permeability oil reservoirs in the Changqing Oilfield. Under the conditions of formation temperature and pressure in the target block, long core experiments and two-dimensional heterogeneous plate large rock model displacement experiments were carried out to explore the effects of permeability and fractures on the swept efficiency of water flooding and CO2 flooding. The swept characteristics and migration law of CO2 in extra/ultra-low permeability reservoirs with fractures and high permeability zones after water flooding are deeply understood. The research shows that: ①The development of micro-fractures is not conducive to the expansion of the swept volume of CO2 flooding. Compared with homogeneous cores, the recovery rate of CO2 miscible flooding after water flooding in one-dimensional fractured long cores is reduced. ② The injection capacity of CO2 miscible flooding is obviously higher than that of water flooding, and the displacement front is obviously more uniform than that of water flooding, which can effectively displace the remaining oil in the matrix. ③ The development of fractures and high permeability zones will lead to uneven distribution of remaining oil after water flooding, and CO2 breaks through earlier along the dominant channel, which seriously affects the swept volume of CO2 flooding. ④ CO2 large PV miscible flooding can still produce oil continuously at high gas-oil ratio and greatly improve the recovery rate.
Keywords: extra/ultra-low permeability reservoirs; fractures and high permeability zones; CO2 miscible flooding; injection-production characteristics

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Poster / 331

Pore Scale Study on Transport Plugging and Displacement Performance Evaluation of a Novel Microencapsulated Polymer Delivery System

Author: Yongsheng Liu[1]

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The key challenge in polymer flooding for reservoir depth profile control is finding a solution to the contradictory relationship between injectivity and effective displacement. One promising approach is the synthesis of microencapsulated polymers with delayed release characteristics, achieved by encapsulating the polymer within microcapsules. However, the accurate assessment of their targeted viscosity enhancement relies on a thorough understanding of the transport plugging and displacement performance of the microencapsulated polymer within porous media.
We evaluated the underlying properties of the microencapsulated polymer. Based on this, microfluidic technology was used to study the flow behavior of the microencapsulated polymer at the pore scale. We utilized a high-speed camera and two high-precision pressure sensors to capture real-time flow images and pressure variations of microencapsulated polymer in a single-contracted PDMS microchannel. Subsequently, we studied the migration characteristics of microencapsulated polymers through parallel microchannels with multiple-width ratios. Finally, we evaluated the oil displacement performance of microencapsulated polymer under different trigger stages using a complex network glass etching model.
The micro-resistance factor was defined as the ratio of the pressure difference between the microencapsulated polymer inside the microchannel and the pressure difference during water injection only. The experimental results demonstrate that the particle size of the microencapsulated polymer can expand up to 3-5 times, while the solution viscosity can increase by more than 25 times. The microencapsulated polymer particles exhibit particle adsorption, blockage, and free passage within the microchannel. The severity of microchannel damage is more pronounced at lower injection flow rates, and the micro-resistance factor of the microcapsules increases with higher concentration. For particle sizes/throats less than 1, the micro-resistance factor is approximately 1. Blockage and adsorption behaviors of capsule particles gradually increase flow resistance, but blockage has a more drastic impact. The microencapsulated polymer tends to enter wider throats in parallel microchannels, but long-term injection causes more severe damage to smaller throats. In terms of micro-flooding experiments, the flooding effect of un-triggered microencapsulated polymer is similar to that of water flooding. As the triggering degree of the microencapsulated polymer increases, the occurrence of the viscous finger-pointing phenomenon significantly weakens, effectively displacing the remaining oil at the edge of the pore model, and enhancing the oil recovery rate by 22.8%.
This study investigated the flow characteristics and oil displacement performance of microencapsulated polymers at the pore-throat scale. This microscopic analysis provides valuable insights into understanding their deep migration and targeted viscosity enhancement. These findings hold great significance for the advancement and practical application of novel oil displacement agents.

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Poster / 332

Extensive pore modelling (XPM) –a coherent framework for multiscale pore network modelling

Authors: Dmytro Petrovskyy[None]; Hannah Menke[1]; Julien Maes[1]; Kamaljit Singh[1]; Tom Bultreys[2]

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It is not uncommon for porous media to span multiple scales of heterogeneity. Geological formations are examples of such complex systems that may act as natural aquifers, hydrocarbon reservoirs or greenhouse gas sequestration units. Application of conventional single scale modelling approaches is not sufficient for representative prediction of flow in such heterogenous permeable media. Instead, a method that marries features of different heterogeneity scales needs to be established and validated.

Three-dimensional digital images of pore spaces are the foundation for numerical pore scale modelling. Depending on the image resolution and the underlying pore structure, voxel data may not be exclusively binary (void or solid), but rather a collection of grey values that indicate under-resolved porous regions. Traditional pore networks have already demonstrated their efficiency and accuracy when modelling single scale macroscopic properties where the porosity is fully resolved. However, rigorous capture of under-resolved heterogeneity remains a difficult task for this class of models.

In our work, we aim to address this shortcoming by introducing an additional set of entities referred to as Darcy nodes that complement existing pore network macro nodes and throats. Physically, the Darcy nodes correspond to under-resolved regions that are characterized by its porosity and permeability. The proposed novelty is the more systematic consistency and flexibility of the Darcy nodes allocation and integration into the existing pore network modelling workflow in comparison to the previously published methods of microlinks (Bultreys et al., 2015) or very large stochastic explicit networks (Jiang et al., 2013). We established a methodology that unites laminar and Darcy flow mechanisms as well as their transitional behaviour, similarly as it is done in the multiscale Darcy-Brinkman formulation, as shown in Figure 1. The accuracy and robustness of our model, as implemented in the XPM (extensive pore modelling) simulator, is confirmed by a comparison with more physically complicated direct numerical simulation modelling results. Finally, our development is open source that is freely and readily available to the wider audience.

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MS12 / 333

Time-Resolved Schlieren Imaging of Pulsatile Flow in Sinuous-Shaped Constricted Pores

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Traditional porous media wave theory, such as the Biot theory and BISQ model, typically rely on the idealized assumption of smooth cylindrical pores. However, in actual reservoirs, pores often manifest as structures with non-smooth walls and varying diameters, where pores and throats alternate, making them far more complex. These real-world conditions pose new challenges, especially in accurately depicting the impact of fluid flow on wave propagation in these complex structures.
In this work we have proposed a new quantitative research method using the sinusoidal-wall tube model to study fluid flow in porous media. This approach is not only applicable in the field of biomechanics, such as in the description of blood flow, but also in rock physics, especially when considering the dispersion and attenuation effects on wave propagation. A highlight of the work is the introduction of the sinusoidal-wall tube structure, adding an extra dimension to pore geometry, thereby differentiating it from previous porous models. Firstly, we have developed a time-resolved Schlieren imaging system to observe fluid flow in the sinusoidal-wall channel. The optical flow method is used to process the Schlieren images, which enabled us to determine the fluid velocity field quantitatively. Base on the observed velocity field, the fluid pressure field is determined by Naiver-Stokes equations. In addition, we used COMSOL software for numerical simulations, which reproduced the presence of countercurrent and vortex flow in the sinusoidal-wall tubes. These experimental observations and numerical results provide strong evidence of new mechanism for wave dispersion and attenuation in porous media. The results of this research may have a profound impact on rock physics, particularly in understanding the behavior of seismic waves propagating in complex porous media.

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MS21 / 334

Non-linear growth of fingers during two-phase flow in porous media

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Invasion of a fluid in a porous medium filled with another fluid immiscible to the injected one produces a wide variety of displacement patterns depending on the fluids' viscosity contrast and the capillary number of the flow. In the case of a low-viscosity fluid advancing through a high-viscosity immiscible fluid, a viscous instability occurs, leading to viscous fingers which have long been assumed to exhibit a linear Laplacian growth behavior. This means that the interface velocities of the advancing fronts depend linearly on the local pressure gradient. This (linear) Laplacian growth behavior is also observed for viscously-unstable fingers observed in continuum Hele-Shaw cells by Saffman and Taylor 1, as well as for diffusion limited aggregates (DLA). However, an experimental study of drainage in a porous Hele-Shaw cell around 20 years ago [2] demonstrated that drainage fingers in porous media can also exhibit non-linearity in the growth in a certain regime. Recently we further investigated this configuration of drainage displacement with a dynamic pore-network model [3] and measured the local growth rate of the fingers as a function of the local pressure drop. We showed that there exists a regime where the two quantities relate nonlinearly with a power-law, which then crosses over to a linear Laplacian growth regime at higher capillary numbers [4]. The origin of this nonlinearity is the disorder in the capillary barriers at the pores [2, 4], and the pore-size distribution, through the distribution of capillary thresholds, controls this non-linearity. In our recent study [4], the pores size distribution was uniform. Here in this talk we will present our further investigations on the sensitivity of these results on the distribution of pore sizes, and how the exponent related to the fingers' growth law depends on the functional form of that distribution.

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1 P. G. Saffman and G. I. Taylor, Proc. R. Soc. London 245, 312 (1958). [2] G. Løvoll, Y. Méheust, R. Toussaint, J. Schmittbuhl and K. J. Måløy, Phys. Rev. E 70, 026301 (2004). [3] S. Sinha, M. Aa. Gjennestad, M. Vassvik and A. Hansen, Front. Phys. 9, 548497 (2021). [4] S. Sinha, Y. Méheust, H. Fyhn, S. Roy and Alex Hansen, arXiv:2312.14799 (2023).

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Poster / **338**

Integrated Workflow of Fracturing-Flowback-Production in Tight Oil Reservoirs with a Focus on Fracturing Fluid Leak-off.

Authors: Wensheng Wu[1]; Xiukun Wang[1]; Yanjie Guo[2]; Wenlong Wu[1]

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

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Corresponding Authors: xiukunwang@cup.edu.cn, 1763683670@qq.com, 1574408557@qq.com, 3088742083@qq.com

Hydraulic fracturing in tight oil reservoirs requires injecting large volumes of fracturing fluid into the formation while only a small proportion of fracturing fluid can flow back during the production phase. The retained fracturing fluid will affect subsequent production. We implement an integrated workflow which simulates fracture propagation through a full 3D simulator and seamlessly docks to an efficient reservoir numerical simulator, then we simulate the injection phase and subsequent production phase using dilation/compaction curves based on fracturing pump injection data and actual production data. The workflow has been successfully applied to a field case in the Daqing Oilfield, China. Our simulations effectively match the oil and water production data and prove our hypothesis that numerous microscale fractures are generated during hydraulic fracturing which cause significant leak-off of the fracturing fluid. The closure of microscale fractures during production phase results in the retention of the fracturing fluid and stable water cut after several months of production.

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Poster / **339**

Research on the microscopic movability characteristics of tight oil with different injection media huff and puff based on NMR technology: A case study of Qinghai Oilfield

Author: Zhuoying Dou[1]

Co-authors: Zhengming Yang [2]; Xianming Li [3]; Chun Feng [4]; Yujianjun Xue [3]; Liang Qiao [3]; Huan Meng [5]; Chenyu Han [6]; Yapu Zhang [2]

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Huff and Puff is an important means to supplement formation energy in the development of unconventional petroleum resources. In this paper, the physical simulation experiments of different injection media huff and puff are carried out by taking the plunged-sample cores of Qinghai oilfield as experimental samples. By means of nuclear magnetic resonance(NMR) technology, the characteristics of oil movability in pore throats of different sizes are quantitatively studied from a microscopic perspective.The influence of soaking time, permeability and wettability on recovery degree is analyzed.The results show that the oil displacement efficiency increases exponentially with the increase of soaking time.The soaking time of water and fracturing fluid huff and puff should not be too long. On the premise of ensuring economic cost, the soaking time of surfactant huff and puff can be appropriately extended. The soaking time of CO2 huff and puff should take into account the pore structure and permeability characteristics of the reservoir, because gas channelling will occur in the reservoir with fractures if the soaking time is longer. Reservoir wettability is of great importance to the development effect of water and surfactant huff and puff. During water huff and puff, imbibition in small pores is dominant in hydrophilic reservoirs, while large pores are mainly movable in lipophilic reservoirs by displacement pressure difference. The movability of small pores is dominant in the early stage and that of large pores in the latter stage. If the surfactant is well performed on the reservoir, the oil film stripping of large pores is faster and predominates. If the surfactant is poor performed on the reservoir, the imbibition of small pores dominates. CO2 huff and puff mainly moves oil in large pores. In a comprehensive comparison, CO2 has the best huff and puff effect and water has the worst huff and puff effect. The oil displacement efficiency of fracturing fluid and surfactant huff and puff depends on the compatibility of the selected surfactant with the reservoir. This study provides a theoretical basis for the selection of injection medium and soaking time for the development of tight oil reservoirs in Qinghai oilfield.

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MS12 / **340**

A New Method for Dynamic Analysis and Predicting Production of Multi - Fractured Horizontal Tight/Shale Oil Wells

Authors: Yanjie Guo[1]; Xiukun Wang[2]; WenSheng Wu[None]; WenLong Wu[2]

[1] *China University of Petroleum, Beijing*

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Corresponding Authors: 3088742083@qq.com, 1574408557@qq.com, xiukunwang@cup.edu.cn, 1763683670@qq.com

Predicting production of tight/shale oil has been attracting people's discussion. In this paper, a new method for dynamic analysis and predicting production of multi-fractured horizontal tight/shale oil wells is provided.
After horizontal well fracturing, the boundary-dominated flow is occurred in the fracture, transient linear in the pressure sweep area is assumed as a series of pseudo-steady states. The appropriate method for historical fitting is selected, and the objective function, inversion parameters, initial values ,adjustable ranges etc is determined. The L-BFGS-B algorithm is used to quickly obtain the specific values of the inversion parameters and complete the historical fitting. On this basis, the prediction of production is completed.
The production data of a well in Daqing oilfield, China is selected to validate this method. The historical fitting effect is very well, and the time is short. The result show that this method has the characteristics of fast calculation speed, high fitting precision and considering multiple inversion parameters.
The novel feature of this method is that the tight/shale oil production prediction model is established on the concept of dynamic sweep, which can realize the rapid prediction of reservoir reconstruction scale and estimated ultimate recovery(EUR). The result of this method can be mutually verified with the numerical simulation result. This paper provides a new method for dynamic analysis and predicting production of multi-fractured horizontal tight/shale oil wells for petroleum engineers.

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Poster / **342**

Two-phase seepage behaviour of hydrate-bearing sediments at pore-scale studied using a CFD approach

Authors: Zhenyuan Yin[1]; Xiaohui Liu[2]; Jidong Zhang[2]

[1] *Tsinghua Univesity*

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Natural gas hydrates (NGH) are considered as the future clean energy in the era of carbon neutrality 1. Seepage behaviour of gas-water flow in hydrate-bearing sediment (HBS) and its controlling factors is significant for developing effective production strategies. The flow patterns and relative permeability are two crucial aspects of the study on two phase flow in HBS, which are influenced by various factors involving pore structure, wettability, hydrate morphology, and fluid properties. Currently, most research is focused on macroscopic permeability, with limited exploration of the flow patterns of gas and water in the presence of hydrates. Additionally, due to the distinct physical properties of hydrate particles such as wettability and phase change [2, 3], experimental methods struggle to observe the interactions between multiphase fluids and the skeleton (sediment + hydrates). Accurate determination of relative permeability is also challenging [4]. This study aims at investigating the characteristics of gas-water flow in the presence of hydrates and constructing an improved method for determining relative permeability based on CFD methods. In microfluidic chip experiments, the morphology and heterogeneous distribution of hydrates, gas-water flow rates, and the wettability of the skeleton were observed. Based on the information obtained from experiments, a geometric model of HBS is constructed. Subsequently, Volume of Fluid (VOF) algorithm using OpenFOAM is applied for simulating two-phase gas-water flow. A steady-state method based on experimental determination of relative permeability was applied to construct gas-water relative permeability curves in numerical simulations.

Fig. 1a presents the observation of pore-scale hydrate morphology and spatial distribution on the microfluidic chip. Hydrate particles with size range of 5- ~500 μm were observed to form within the pores, indicating a pore-filling type. Fig. 1b is the generated numerical model of HBS. Fig. 1c-d shows the CFD simulation of gas-water flow behaviours in HBS. The influence of hydrate saturation and contact angles on the dynamic distribution of gas and water in pores were investigated. When the water-particle contact angle is small, the gas phase displacement exhibits a fingering pattern, forming distinct preferential flow channels. As the contact angle increases, the gas phase transitions into a discontinuous state, causing some water to be retained within the pores. Fig. 2a depicts the variation of water saturation and inlet-outlet pressure drop over time with steady-state method. Various water saturation are achieved by setting different ratios of inlet gas to water flow rates until reaching the final stable state. The effective permeability of gas and water is then calculated according to Darcy's law (as shown in Fig. 2b).

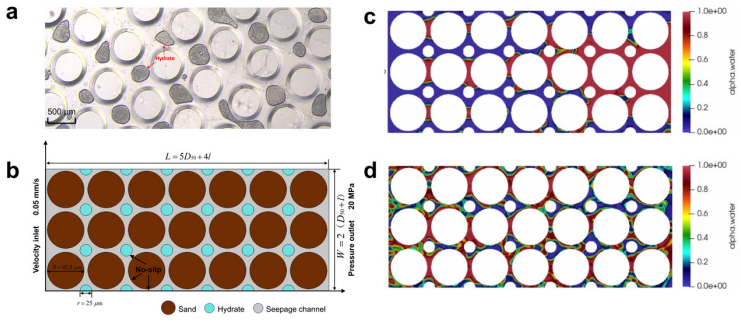

Figure 4:

Fig. 1. (a) CH4 hydrate morphology and spatial distribution on the microfluidic chip. (b) Generated numerical model of HBS. (c-d) gas-water flow patterns in simulations.

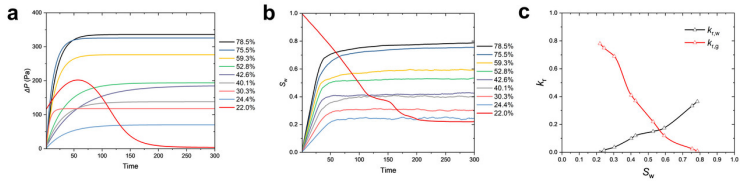

Figure 5:

Fig. 2. (a) water saturation and (b) inlet-outlet pressure drop over time. (c) gas-water relative permeability curve.

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1 Z. Yin, P. Linga, Methane hydrates: A future clean energy resource, Chinese Journal of Chemical Engineering, 27 (2019) 2026-2036. 2 J. Zhang, X. Liu, D. Chen, Z. Yin, An investigation on the permeability of hydrate-bearing sediments based on pore-scale CFD simulation, International Journal of Heat and Mass Transfer, 192 (2022). [3] J. Zhang, Z. Yin, Q. Li, S. Li, Y. Wang, X.-S. Li, Comparison of fluid production between excess-gas and excess-water hydrate-bearing sediments under depressurization and its implication on energy recovery, Energy, 282 (2023) 128315. [4] G. Gong, G. Zhao, W. Pang, M. Yang, B. Chen, J.-n. Zheng, Review of hydrate-bearing sediment permeability for natural gas hydrate exploitation: Measurement and application development, Journal of Petroleum Science and Engineering, 220 (2023) 111217.

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MS17 / 343

Pore-scale study of CH4 hydrate morphology and kinetic behavior by high-pressure microfluidics

Authors: Jidong Zhang[1]; Xiaohui Liu[1]; Zhenyuan Yin[2]

[1] *Tsinghua University*

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Corresponding Authors: zhang-jd21@mails.tsinghua.edu.cn, zyyin@sz.tsinghua.edu.cn, liuxh21@mails.tsinghua.edu.cn

Natural gas hydrates (NGH) are ice-like crystalline substances that consist of water molecules acting as host and methane guest molecules and formed at low temperature and high pressure 1. Methane hydrate (MH) has been considered a promising future energy source due to its vast resource volume and high energy density. Understanding the behavior of MH formation and dissociation at pore-scale and the effect of MH distribution on the gas-liquid two phase flow is of critical importance for designing effective production strategies from NGH reservoirs 2. The phase change of

NGH from a gas-liquid two-phase system, the evolution of NGH morphology, and the distribution of NGH at the pore-scale provide critical insights into understanding the underlying thermal-hydraulic-mechanical-chemical process [3]. Additionally, depressurization method has garnered significant research attention over the past decades and is widely considered the most promising approach due to its high energy efficiency [4]. This warrants the development of novel experimental techniques to provide direct visual evidence for MH formation and depressurization-induced dissociation and the evolution of gas bubbles in pores.

In this study, we devised a novel high-pressure microfluidic chip apparatus that is capable of direct observation of MH formation and dissociation behavior at pore scale. Fig. 1a shows the experimental apparatus for pore-scale investigation on the microfluidic chip. The entire apparatus consists of four major components: a) a confining pressure holder; b) an etched microfluidic chip, as shown in Fig. 1b; c) a constant flow-rate syringe pump; d) a high-resolution charge-coupled device camera. MH nucleation and growth were conducted under same conditions with Shenhu Sea, South China Sea (P = 15.0 MPa, T = 276.2 K). Depressurization was used to induce MH dissociation at three different BHP of 12.0, 10.0, 8.0 MPa with constant pressure drawdown rates of 7.0 MPa/h at T = 287.7 K.

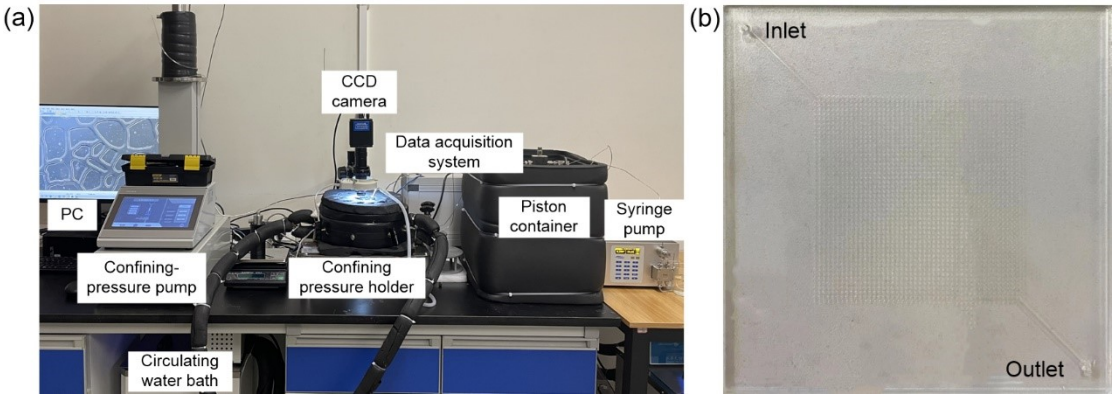

Figure 6: enter image description here

Fig. 1. (a) picture of the in-house made high-pressure microfluidic; (b) the microfluidic chip used in this study.

Fig .2 shows the evolution of P and T, and MH morphology and gas bubbles during MH dissociation under depressurization. Our experimental results reveal that two types MH formation mechanisms co-exist in pores: (a) porous-type MH formed from CH4 gas bubbles; and (b) crystal-type MH formed from dissolved CH4 gas. Crystal-type MH is relatively stable and its dissociation pressure is lower than that of porous-type MH. MH dissociation in the pores produce obvious aggregation and coalescence, and converge into a continuous gas phase flowing within the pores under depressurization. The experimental results from our study aim to provide a direct pore-scale observation of NGH formation and dissociation and provide a fundamental understating of gas-liquid two phase flow.

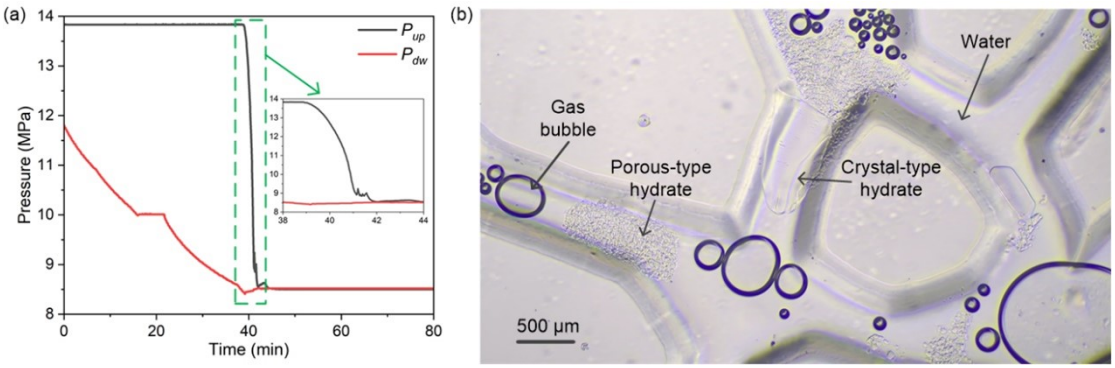

Figure 7: enter image description here

Fig .2. (a) Evolution of P of microfluidic chip; and (b) evolution of MH morphology and gas bubbles during MH dissociation under depressurization.

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1 Yin Z, Khurana M, Tan HK, Linga P. A review of gas hydrate growth kinetic models. Chemical Engineering Journal. 2018; 342:9-29. 2 Zhang J, Yao Y, Yin Z. Fluid production from NGH reservoir: fundamental physics, numerical model, and reservoir simulation. Challenges and Recent Advances in Sustainable Oil and Gas Recovery and Transportation: Elsevier; 2023. p. 53-80. [3] Mahabadi N, Jang J. Relative water and gas permeability for gas production from hydrate-bearing sediments. Geochemistry, geophysics, geosystems. 2014;15(6):2346-53. [4] Zhang J, Yin Z, Li Q, Li S, Wang Y, Li X. Comparison of fluid production between excess-gas and excess-water hydrate-bearing sediments under depressurization and its implication on energy recovery. Energy. 2023;282, 128315.

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Poster / 344

A Semi-Analytical Method for Predicting Three-Phase Flow Production in Condensate Gas Reservoirs

Author: Yaxian Wang[None]

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During the condensate gas production process, condensate oil will precipitate, the phase state will change, and the seepage mechanism is complex. There are currently few analytical models for multiphase flow. Therefore, a semi-analytical method for three-phase flow production in condensate gas reservoirs is studied. Considering the vaporized oil ratio, solution gas-oil ratio, and solution gas-water ratio, the differential equations of oil saturation and water saturation are obtained through the two expressions of each of the production gas-oil ratio and the production water-oil ratio. The relationship between saturation and pressure can be solved. Given the gas rate, based on the three-phase material balance equation, the average reservoir pressure at any point in time is obtained, and then the production gas-oil ratio and production gas-water ratio are obtained, so as to obtain the changes of oil rate and water rate over time. From the pseudo steady state gas rate formula, the bottom hole flowing pressure can also be obtained. Compared with the numerical simulation results, the correctness of this method is verified. This method considers the three phases of oil, gas, and water, including dissolved gas and volatile oil, and provides an efficient semi-analytical approach for production dynamic analysis, which facilitates the practical application of petroleum engineers in condensate gas reservoirs.

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Shahamat, M. S., and C. R. Clarkson. "Multi-Well, Multi-Phase Flowing Material Balance." Paper presented at the SPE Unconventional Resources Conference, Calgary, Alberta, Canada, February 2017. doi: https://doi.org/10.2118/185052-MS. Marhaendrajana, T., Ariadji, T., and A. K. Permadi. "Performance Prediction of a Well under Multiphase Flow Conditions." Paper presented at the SPE Asia Pacific Oil and Gas Conference and Exhibition, Jakarta, Indonesia, September 2003. doi: https://doi.org/10.2118/80534-MS.

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MS17 / 345

Domain decomposition physics-data combined neural network for parametric reduced order modelling of fluids

Author: Xinyu Pan[1]

Co-author: Dunhui Xiao [1]

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Reduced Order Modelling (ROM) is a widely used method in various engineering such as fluids, porous media, reservoir modelling and so on. This paper proposes a novel domain decomposition physics-data combined neural network(DPDCNN) approach to construct a ROM. In this method, Proper Orthogonal Decomposition (POD) is applied to each sub-domain to reduce dimensionality. Neural network is then used to predict POD coefficients of each sub-domain. The physical equations are incorporated into the loss function. In this domain decomposition method, several additional conditions are enforced at the interferes to ensure the overall continuity of physical solutions such as averaging solutions at neighbourhood, next time levels' values and derivative terms of the PDEs. The performance of this newly domain decomposition method is compared against the model without domain decomposition. The capability of this method is tested using a number of parametric nonlinear problems such as KDV equation in a regular domain, two-dimensional Kovasznay flow, and the two-dimensional Incompressible Navier–Stokes equation.

The results indicate that the proposed methods offer an economically effective means of constructing a reduced model for parameterized PDEs through machine learning. Particularly in specific parameter ranges, especially when distinct physical phenomena regions are prominent, the method outperforms the model without domain decomposition, demonstrating excellent performance on several challenging problems.

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Poster / 346

Dynamic Effects on Solute Transport in an Unsaturated Soil

Author: Luwen Zhuang[1]

Co-authors: Han Zhu [1]; S. Majid Hassanizadeh [2]

[1] *Sun Yat-sen University*

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The influence of flow regime and soil saturation on solute transport processes is significant, yet the associated effects have not been adequately addressed. To address this gap, we conducted three sets of solute transport experiments in a sandy soil, complemented by numerical modeling, under both steady-state and dynamic drainage conditions. The results from steady-state experiments revealed a non-monotonic relationship between dispersivity and saturation.Both classical advection-dispersion and dual-porosity (mobile-immobile) type transport equations were used to simulate the measurements. The fitted well defined dispersivity -saturation function was employed to the simulations of dynamic experiments. Taking into consideration the dynamic capillarity effect, our model accurately simulated solute transport processes and flow. Contrary to previous reports, our findings suggest that the flow regime does not significantly impact the dispersivity of solute transport.

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MS07 / **347**

A Hybrid-Dimensional Stokes–Brinkman–Darcy Model: Derivation, Analysis and Validation

Author: Linheng Ruan[1]

Co-author: Iryna Rybak [1]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*

Corresponding Authors: iryna.rybak@ians.uni-stuttgart.de, linheng.ruan@ians.uni-stuttgart.de

Coupled free-flow and porous-medium systems have received rising attention in recent years due to their broad applications in the environment, biology, and industry. A suitable coupling concept should be applied to characterize fluid behavior between the free flow and porous medium. However, the majority of coupling conditions are restricted to flows parallel to the fluid-porous interface.

In this talk, we present a hybrid-dimensional model for coupled free-flow and porous-medium systems which is suitable for arbitrary flow directions. We consider a narrow transition region between these two flow systems that stores and transports mass, momentum, and energy. The proposed hybrid-dimensional model incorporates the Stokes equations in the free flow, the averaged Brinkman equations along the transition region, and Darcy's law in the porous medium. Appropriate transmission conditions are considered between the three regions. The well-posedness of the developed hybrid-dimensional model is proven. The model is validated against the pore-scale resolved simulations and compared with other coupling concepts. Numerical simulation results demonstrate the advantages of the proposed model in comparison to the coupling concepts available in the literature.

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MS03 / **348**

Modeling of micro-particle transport in supercritical CO2 over rough fractures

Authors: Qianqian ZHOU[None]; Bin Wang[1]; Haizhu Wang[None]; Mengmeng Zhou[None]; Zhichao Yang[None]; Yong Zheng[None]

[1] *China University of Petroleum - Beijing*

Corresponding Authors: zqq00325@163.com, 1061435301@qq.com, zhoumm@cup.edu.cn, bin.wang@cup.edu.cn, wanghz@cup.edu.cn, yangzhichao0625@163.com

SC-CO2 (supercritical carbon dioxide) has attracted much attention in subsurface engineering process, such as CO2 sequestration, enhanced oil recovery and geothermal development. Using micro-particle as proppant in SC-CO2 fracturing is a new fracturing technology in unconventional oil and gas reservoirs. Despite the multiphase flow of SC-CO2 in porous media has been widely studied in recent years, the transport of micro-particles in SC-CO2 over fractures still need further research. In this study, a coupled computational fluid dynamics and discrete element method (CFD–DEM) approach is used to study the transport behavior of micro-particles with SC-CO2 over rough natural fractures. Rough fracture geometries are generated with the geostatistical simulator Synfrac. The difference in the particle transport characteristics between SC-CO2 and slick-water are demonstrated. The effects of fluid properties, particle parameters, and fracture morphology on micro-particle carrying behaviors in rough fractures were discussed. Results show that particle-carrying performance depends on fluid viscosity and flow rate. Larger critical settling velocity of particles in low viscosity SC-CO2 leads to the formation of sand dune at the bottom of fractures. Micro-particles are prone to form a multi-layer's sand dune with high particle concentration. Also, the presence of vortices in SC-CO2 around a rough fracture surface leads to the suspension of micro-particles, particularly when the flow field is subjected to high injection rate and high Reynolds number. This ultimately results in a wider distribution of micro-particles in SC-CO2 within the fracture compared to water. Due to the particle accumulations on the sand bed surface, fracture apertures is reduced and leads to fast flow velocity. The turbulent flow regions of CO2 fluids are generated. In the vicinity of high Reynolds flow regime, the flow field enhances the suspension capacity of particles. Turbulent flow at fracture junctions helps to deliver particles into deeper and farther of natural fractures in low viscosity SC-CO2 fluids by disturbing the movement of sand dune. The overall findings provide a greater understanding of transport behaviors of micro-particle with SC-CO2 over rough fractures underground.

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Poster / 349

Pore-scale Modeling and Numerical Simulation for Viscoelastic Emulsion Flow

Authors: Haoran Cheng[1]; Rui Huang[2]

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In this study, a body force driven two-phase fluid flow in porous media is numerically simulated by weakly compressible smoothed particle hydrodynamics, a Lagrangian mesh free particle method. The dispersed phase consists of viscoelastic emulsive droplets and is assumed to obey Oldroyd-B rheological model. The background phase is a Newtonian fluid. The interfacial tension between two phases and the wettability between fluids and solid boundaries are evaluated by pairwise force model. Different flow velocity, viscosity ratio and Weissenberg number are investigated. All simulations are implemented on GPU to achieve high efficiency.

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MS17 / 351

Advanced 4D Imaging of Shales at Micro- to Nano-scale: Investigating the time-lapse evolution Under Subsurface Thermal, Hydrological, Mechanical, and Chemical Conditions

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Mudstones and shales are the source of unconventional oil and gas reservoirs, as well as the primary control on the sealing efficiency for subsurface storage applications (e.g. energy, CO2, H2, waste). However, their fine-grained and heterogeneous nature makes their full characterisation highly challenging. Here we demonstrate the multi-scale and dynamic imaging approaches that can help meet these challenges and discuss limitations and future opportunities.

Microstructures can be characterised at scales from sub- nm (<1 nm) to over 1 m, using multi-scale and multi-model imaging approaches [1-3], including X-ray tomography, Focused Ion Beam Scanning Electron Microscope and Transmission electron microscopy tomography. The majority of pores in mudstones/shales range from 0.2 nm to 3μm, and we have documented 4 major types with 3 distinct size distributions [4]. Based on the REV analysis, pore sizes, types and distribution can be upscaled via three stages from sub-nm to cm-scale[5]. The permeability is pressure dependant, ranging from 1.0×10-17 to 1.0×10-22m2 [3, 5]. CO2 adsorption is 3-7 times higher than CH4 and over 10 times higher than H2 [6]. Image based modelling has demonstrated that the non-Darcy effects (e.g., slip flow and Knudsen diffusion). Adsorption/desorption and surface diffusion takes major controls over time after injection [7].

Dynamic imaging of mudstones/shale has provided the opportunity to characterise the thermo-hydro-mechanical-chemical (THMC) properties and the coupling mechanism in mudstones/shales to investigate the sealing ability under realistic reservoir conditions. These include high temperature

(from less than 10 ℃ up to 1000 ℃) [8], high pressure (e.g. confining pressure, indentation, torsion, deformation and fractures; up to 65 MPa) [9], fluids (e.g. diffusion, adsorption, flowing through, multi-phase flow) [10] and complex chemistry environment (brine and drilling fluids) [11]. Based on the dynamic behaviours observation and quantification, It can be concluded that mudstone/shales with horizontally thin-layered laminations, few fractures and less reactive minerals may act as the best caprocks.
Whilst the above has led to an improved understanding of shale/mudstone microstructure under static and dynamic conditions, significant challenges still remain regarding representivity and up-scaling, experimental analysis at subsurface-realistic temperatures, pressure and chemistry, accurate estimations of the long-term behaviours and the proper monitoring techniques.
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MS01 / **352**

OpenWorkFlow - Development of an open-source synthesis-platform for safety investigations in the site selection process

Author: Olaf Kolditz[1]

Co-authors: Christoph Lehmann [2]; Thomas Nagel [3]

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The search for suitable sites for the safe disposal of radioactive waste, a prerequisite for phasing out nuclear energy, is a major scientific, technical and political challenge on which intensive work is being done worldwide. Numerical models for safety investigations for site selection will also play an important role in the endeavour. The OpenWorkFlow project, which was initiated by the Bundesgesellschaft für Endlagerung (BGE), is creating a novel, open synthesis platform for the virtualization of repository systems. The simulation platform will be used both for the evaluation of far-field and near-field processes to support the site selection process and later for the geotechnical design of

repository systems. Continuity and innovation are two basic principles of our development philosophy. Through continuous scientific development, the platform will always be at the cutting edge of science and technology and help to shape it. In addition, OpenWorkFlow is developed using the latest IT and digitization methods and the software concept is continuously adapted. As the name suggests, OpenWorkFlow is an open workflow platform, developed as an open source project based on the FAIR principles and an invitation to the community to participate.

Source:
Christoph Lehmann, Lars Bilke, Jörg Buchwald, Nico Graebling, Norbert Grunwald, Julian Heinze, Tobias Meisel, Renchao Lu, Dmitri Naumov, Karsten Rink, Ozan Özgür Sen, Philipp Selzer, Haibing Shao, Wenqing Wang, Florian Zill, Thomas Nagel, Olaf Kolditz (2024): OpenWorkFlow - Development of an open-source synthesis-platform for safety investigations in the site selection process, Grundwasser, in print

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Christoph Lehmann, Lars Bilke, Jörg Buchwald, Nico Graebling, Norbert Grunwald, Julian Heinze, Tobias Meisel, Renchao Lu, Dmitri Naumov, Karsten Rink, Ozan Özgür Sen, Philipp Selzer, Haibing Shao, Wenqing Wang, Florian Zill, Thomas Nagel, Olaf Kolditz (2024): OpenWorkFlow - Development of an open-source synthesis-platform for safety investigations in the site selection process, Grundwasser, in print

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MS09 / 353

The pinning dynamics of a non-wetting droplet penetrating a permeable substrate

Authors: Chiyu Xie[None]; Hongqing Song[1]; Junming Lao[None]

Co-authors: Bin Pan [2]; Hongen Yang [3]; Lin Liu [3]

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Problem statement
The droplet penetration plays an essential role in various fields such as inkjet printing, fuel cells, oil and gas development, new material preparation, and enhanced heat transfer. The functions of non-wetting droplets are used to be limited due to the capillary resistance to its penetration into micropores, but the application of magnetic, electric, acoustic and optical forces, has overcome the limitation. However, the dynamics of the penetration and contact line pinning of non-wetting droplets remain unclear.

Methods
The contact line pinning mechanisms of a non-wetting droplet penetrating a permeable substrate are theoretically explained by considering the force balance of volumetric force, capillary force, and pinning and depinning forces. We propose two dimensionless numbers, Bo* - the ratio of the volumetric force to the capillary force, and Ct - the ratio of the depinning force to the pinning force, to establish a phase diagram that quickly determines the droplet penetration patterns. We further perform a series of lattice Boltzmann (LB) simulations, and the results match well with our theoretical analysis.
Results
The time evolutions of the contact area diameter Dc, the droplet height h, the penetrated droplet volume percentage Sp, and the apparent contact angle θ are derived as illustrated in Figure 1, in which the contact angle dynamics during contact line pinning and shrinking are further clarified. For Bo* ≤ 1, the droplet will not penetrate the substrate; for Bo* > 1 and Ct ≤ 1, the droplet will penetrate with a pinned contact line; for Bo* > 1 and Ct > 1, the droplet will penetrate with contact line shrinking. The phase diagram that quickly determines the droplet penetration patterns is exhibited in Figure 2.
Discussions and Conclusions
The penetration dynamics of a non-wetting droplet into a permeable substrate are studied both theoretically and numerically, with a special focus on the contact line pinning mechanisms. The lattice Boltzmann simulations are performed and show excellent agreements with our theoretical derivations and intuitively illustrate the dynamic penetration processes.
We propose two dimensionless numbers: a modified Bond number Bo* and a new dimensionless number Ct. These two numbers are applied to establish a phase diagram using that determines the penetration patterns and pinning conditions of the droplet: if Bo*≤1, the droplet will not penetrate the substrate; if Bo*>1 and Ct≤1, the droplet will penetrate with a pinned contact line; if Bo*>1 and Ct>1, the droplet will penetrate with contact line shrinking. For the droplet penetration mode with contact line shrinking, we also find the contact angle change can be divided into three patterns: the constant contact angle, the contact angle rebound, and the contact angle decrease.
This work successfully explains the pinning mechanisms of the penetrating non-wetting droplet found in experiments, moreover, the phase diagram offers a quick evaluation of the droplet penetration patterns, and provides new guidelines to achieve better performance for many applications.

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MS08 / **354**

Fingering Instability During Mixing-Driven Precipitation Flow: Experiments and Simulations

Authors: Benzhong Zhao[1]; Negar Shahsavar[1]; Xiaojing Fu[2]

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Reactive flows in porous media that results in precipitation of solids are ubiquitous in a wide range of applications. Laboratory studies focusing on microscopic changes of the porous media have elucidated the complexity of the precipitation patterns due to the highly nonlinear coupling between advection, diffusion, reaction, and the intrinsic heterogeneity of the pore geometry and mineralogy. Here, we study the displacement of aqueous solutions of calcium chloride by sodium carbonate in a Hele–Shaw cell where the two fluids react, upon mixing, to form calcium carbonate precipitates. We examine the case of equal reactant concentrations in detail via high-resolution imaging, which reveals a variety of precipitation patterns at different injection rates and reactant concentrations. We find that reaction along the moving fluid–fluid interface forms a precipitation band in the form of particle suspensions, whose width and particle concentration are controlled by the injection rate. This injection rate dependent behavior arises due to particle–particle agglomeration in the precipitation band. Higher injection rates generate larger particles and lower suspension mobility, resulting in miscible viscous fingering at the precipitation band. Critically, fingering has important control over the growth of precipitation amount in time, which is diffusive with time in the absence of fingering but is linear with time in the presence of fingering. Furthermore, we show that the precipitates uniformly deposit onto the top and bottom surfaces of the Hele–Shaw cell as a thin particle layer at low injection rate, but they form large particle islands at high injection rates. We develop a novel reaction-diffusion-convection model that not only captures the phenomenology of the precipitation and deposition process, but also the scaling of the temporal precipitation amount.

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MS17 / **355**

Experimental study on pressure-increased water injection by nuclear magne

Author: Renyuan SUN[1]

Co-authors: Peng GU [2]; Bo LIU [3]; Dongdong LIU [2]

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

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Waterflooding is one of the key technology for oilfield development. Reasonable injection and production design is very important for efficient development and enhanced oil recovery. The pore size, oil and water saturation of reservoirs are different, and the remaining oil saturation occurrence mode is different. How to effectively start the remaining oil and which pores start the remaining oil is one of the problems concerned in oilfield development. Core displacement test is used to develop

water injection in different pressure gradients. The effects of injection and production pressures, permeability and different pressure gradient on oil recovery factor and water-cut were evaluated by means of nuclear magnetic resonance test. The results show that oil recovery factor increases first and then decreases with the increase of injection rate. Oil recovery factor increases first and reaches a maximum at 8mL/min, and the total recovery factor of high, middle and low permeability cores decreases in turn. The recovery factor increased to the highest when the pressure was increased to 8mL/ min. The pore structure of the core is dominated by small pores and large pores, while there are a few medium pores, and large pores are the main contributing areas of oil production. For low permeability core, the oil in small pores is mainly moved by pressure increasing, while for medium and high permeability core, the oil in large pores is mainly moved for pressure increasing.

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MS11 / 356

Effectiveness of CO2 microbubble method for enhanced oil recovery in fractured reservoirs

Authors: Baocai Tong[1]; Donglei Liu[1]; Lanlan Jiang[1]; Yongchen Song[1]

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Recently, CO2 microbubbles (MBs) injection has become an important method to increase oil production in fractured reservoirs and reduce greenhouse gas emissions due to its unique physicochemical properties. The stability and size distribution of MBs as well as their flow behavior at the pore scale are key to improving the displacement efficiency and regulating the performance. In this study, a high-speed homogenizer was used to prepare CO2 MBs dispersions, and the effectiveness of this method for enhanced oil recovery in fractured reservoirs was investigated by microfluidic experiments. The results showed that the microbubbles consisted of a special three-layer structure and existed independently in the liquid phase without aggregating with each other. Moreover, the prepared MBs had a size range of 9.73-75.53 μm with an average diameter of 38.73 μm. Compared to the low sweep area resulting from inadequate mobility control of water injection, MBs injection can significantly increase flow resistance to achieve maximum sweep efficiency and oil recovery of 93.02% and 91.04%, respectively. This study demonstrates that CO2 MBs can be used as a promising method for enhanced recovery in oil reservoirs.

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Simulation of reactive dissolution core and pore scale in carbonate reservoir based on DBS equation

Author: Hongfeng Zhang[None]

Co-authors: Jun Yao [1]; Yongfei Yang [1]

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Mineral trapping has attracted much attention because it can realize permanent safe and effective CO2 sequestration, the essence of which is that H+ generated by dissolving CO2 into water reacts with rocks. There are many factors affecting this reaction, and it is important to accurately characterize the dissolution mode and the dissolution law under different combinations of influencing factors. In this paper, based on the Darcy-Brinkman-Stokes method coupling fluid flow, mass transfer, reaction, and rock structure changes, core-scale and pore-scale models were established to study the acid-rock reaction process. Firstly, the effects of pH and chemical reaction constants on the dissolution process were analyzed, and the dissolution mode and the change rule of pore seepage properties under different combinations of pH and chemical reaction constants were determined. The core erosion patterns under different combinations of pe number and Da number were also investigated, and the core erosion patterns were mapped. Subsequently, the simulation was focused on the pore scale, and the dissolution process in three-dimensional pores was investigated, and different dissolution patterns and patterns of porosity, permeability and specific surface area were seen in micrometer-scale pores, and it was found that the pore permeability patterns under different dissolution patterns were different, and that the decrease of pH could effectively accelerate the dissolution rate, but it would not change the dissolution pattern of the rock.

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MS12 / **358**

Hydro-mechanical coupling analysis method for dynamic response of coral reef island airport foundation under aircraft load

Author: Ning Zhang[1]

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Airports on South Pacific islands are often built on coral sand foundations. The coral sand particles of the foundations are characterized by high porosity, irregular shapes, and particle fragile. The hydro-mechanical coupling responses of the coral sand foundation caused by the cyclic aircraft load are still unknown. This research focuses on the increase in porous pressure and softening of the sand structure of the foundation, which are the dominant factors affecting the long-term stability of the airport foundation. To obtain those factors, a hydro-mechanical coupling simulation was conducted with a typical foundation FEM model composed of the runway, foundation, and base rock. The Biot dynamic consolidation theory and the viscoelastic plastic constitutive model of the coral sand were applied in the simulation. The aircraft moving load was calculated via the International Flatness Index (IRI) method. The response characteristics of the coral island airport foundation under the long-term aircraft moving loads were simulated, and the evolution of foundation damage and long-term settlement during airport operation were obtained. The long-term stability evaluation of typical coral island airport foundations was obtained through the deformation control theory.

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MS06-B / **359**

The Impact of System Softness on Haines Jumps in Porous Media

Author: Zhonghao Sun[1]

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Haines jump is an interfacial instability characterized by fluid redistribution and sudden pressure changes. It is a pore-scale phenomenon that occurs during displacement front movement and is widespread in multiphase flow processes in porous media. It is an essential physical process that affects fluid distribution, flow regimes, and displacement efficiency. Previous studies have shown that Haines jump is an instability phenomenon taking place in a soft system comprised of entrapped gas bubbles, deformable porous media, and interacting menisci. This study aims to further investigate the impact of system softness on Haines jumps in porous media.
We conduct fluid displacement experiments in polydimethylsiloxane (PDMS) microfluidic chips and analyze the pressure signature and flow phenomena during Haine jumps. A syringe pump (Chemyx Fusion 200) maintains a constant injection rate, and a microscope (ZEISS) records the displacement process. A microfluidic pressure sensor (Fluigent) placed at the inlet measures the pressure change. The system softness is controlled by adjusting the volume of an air bubble entrapped near the inlet. The PDMS microfluidic chip is fabricated using the standard soft lithography technique. De-ionized water and ethanol are used as wetting fluids, and air is the nonwetting fluid. The impact of system softness is investigated in three conditions: single pore throat, pores in series, and pore network.
Results show that system softness affects the position where Haines jumps occur at the pore throat and the distance of the interface jump. The interface jumps a longer distance when the entrapped air bubble volume increases. It also takes a longer time for the interface to reach the unstable point. An analytical model is proposed to explain the pressure change and interfacial jump at the pore throat and matches well with the experimental observation. In cases of pores in series, the pressure signature shows a "saw"shape where sudden pressure changes and interface jumps occur at pore throats. However, the interface can jump across more than one pore as the system softness increases. As the system softness affects the magnitude of Haines jumps, it also influences the snap-offs, entrapped fluid saturation, and displacement efficiency in pore networks.
In summary, the influence of system softness on Haines jumps and its impact on fluid displacement are analyzed in detail in both single pores and pore networks. Our experiments provide insights into the pore-scale physics of Haines jumps and the impact of Haines jumps on multiphase flow in porous media.
Keywords: Haines jump, porous media, microfluidics, instability, multiphase flow, interface

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Network Model for Low-Permeability Fractured Oil Reservoirs

Author: Guoyu Qin[1]

Co-authors: Liming Zhang [1]; Xia Yan ; Kai Zhang [2]; Yongfei Yang [2]; Jun Yao ; Qinyang Dai

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The pore structure and fluid flow characteristics of low-permeability fractured oil reservoirs are highly intricate, posing a challenge for establishing full-scale numerical simulation models. Describing the fracture system is a key difficulty in developing such reservoirs. Currently, commonly used approaches involve creating equivalent media models, dual-porosity models, and discrete fracture models, embedding them into full-scale simulators. However, these methods often incur high computational costs during simulation and optimization. Therefore, developing a simplified model that ensures both accuracy and rapid computation is crucial for reservoir development. In this study, we introduced a network model where wells are connected by two flow pipes—one representing the matrix system and the other being the fracture system. The inter-well connection network is initialized based on distance, angle, and maximum connection quantity, with volume and transmissibility values assigned to each flow pipe. A mathematical model is established using material balance equations, incorporating fluid flow characteristic equations for both matrix and fracture systems. Through example testing, the proposed model demonstrates compatibility with full-scale reservoir models while achieving computational speeds several times faster.

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MS13 / 363

Multicompotent image-based modeling of water flow in mixed wet shale nanopores

Author: Xiangjie Qin[1]

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Shale contains abundant multi-component nanopore spaces with different wettability. Water flow in multi-component nanoporous systems is still unclear due to the effects of complex pore throat topology and heterogeneous wettability, which limits knowledge of hydraulic fracturing for enhanced hydrocarbon recovery. This work reconstructs single-component (i.e. clay, organic, inorganic matter) and multi-component coupled nanoporous media utilizing image fusion technique. A numerical model for water flow in complex nanoporous systems is developed considering the heterogeneous wettability, slip effect, and effective viscosity. The water flow mechanisms in single and

multi-component heterogeneous wetting systems are systematically analyzed. Results show that the enhancement factor increases exponentially, and the tortuosity increases with increasing contact angle. The flow is weakened under strongly hydrophilic conditions, and the enhancement factor is linearly negatively correlated with specific surface area. Under hydrophobic conditions, a small throat aspect ratio corresponds to a large enhancement factor, and quasi-circular pores limit the enhancement. Due to the differences in pore throat size and wettability, water flow is weakened in clay pores and enhanced in organic pores. For the multi-component heterogeneous wetting system, the global flow is enhanced compared to no slip and uniform wetting systems; the velocity is enhanced non-uniformly due to the altered pathways in organic pores; the flow is slightly weakened in the clay pores. This work provides a numerical perspective for water flow in shale multi-component nanoporous systems.

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MS10 / 365

Real-world image super-resolution for digital rock analysis

Authors: Shaohua You[1]; Qinzhuo Liao[1]; Zhengting Yan[1]; Yutian Ma[1]; Gensheng Li[1]

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The porous media community extensively utilizes digital rock images for core analysis. High-resolution digital rock images that possess sufficient quality are of great importance, but are sometimes difficult to obtain and suffer from high cost. Super-resolution (SR) approaches enhance the resolution of digital rock images, and provide improved visualization of fine features and structures, aiding in the analysis and interpretation of rock properties, such as pore connectivity and mineral distribution.

However, the majority of the existing SR methods are trained on fabricated datasets, in which the low-resolution images are created by applying a basic and consistent degradation, e.g., bicubic downsampling, to their high-resolution equivalents. And the actual low-resolution images captured from real-world scenarios could be different from the fabricated low-resolution images. Consequently, the SR models trained on fabricated data demonstrate reduced effectiveness when employed in practical situations.

In this study, we construct a real SR dataset by capturing paired low- and high-resolution images of the same rock samples using the scanning electron microscope (SEM) and computed tomography (CT) at multiple resolutions. Additionally, an image registration algorithm is developed to progressively align the image pairs at varying resolutions. Our experiments demonstrate that applying the

bicubic downsampling to the high-resolution images, although widely used, is not always a good approximation of the real low-resolution images. The reason behind this can be partially explained by the mechanism in the SEM and CT techniques.

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MS23 / 366

Pore-scale investigation of forced imbibition in natural rocks through interface curvature and pore topology analysis

Author: Jianchao Cai[1]

Co-author: Xiangjie Qin [2]

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Forced imbibition, which involves the invasion of a wetting fluid in natural rocks, plays an important role in efficient development of hydrocarbon resources and geological storage of carbon dioxide. However, the interface dynamics influenced by complex topology lead to non-wetting fluid trapping, particularly the underlying mechanisms under viscously unfavorable conditions remain unclear. This work reconstructs digital rocks of sandstone to simulate forced imbibition by direct numerical simulation methods. The interface dynamics and fluid-fluid interactions are investigated through transient simulations, while the pore topology metrics are introduced to analyze the impact on steady-state residual fluid distribution obtained by a pseudo-transient scheme. Results show that the cooperative pore-filling process promoted by corner flow is dominant at low capillary numbers; the inlet pressure, mass flow, and interface curvature are unstable, corresponding to complicated interface dynamics and higher residual fluid saturation. The interface curvature gradually increases during forced imbibition, with the pore-filling mechanisms involving the cooperation of main terminal meniscus movement and arc menisci filling. Complex topology with small diameter pores may induce instability of interface curvature. Residual fluid saturation is negatively correlated with porosity and pore throat radius, and positively correlated with tortuosity and the aspect ratio associated with pore throat radius. A large mean coordination number characterizing global connectivity promotes imbibition. While the high connectivity characterized by standardized Euler number corresponding to small pores has a high probability of non-wetting fluid trapping.

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MS03 / **368**

Visualization and Quantification of micro-particle transport in rough fractures

Authors: Yaochen Zhang[1]; Yunpeng Zhang[2]; Bin Wang[3]; Haizhu Wang[2]; Mengmeng Zhou[2]; Qianqian ZHOU[None]

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Particle transport in rough natural fractures has seen diversified potentials and applications in environmental engineering and resource development engineering.
Despite intensive and outstanding research on their transport phenomena, the impact of surface attachment and confined space of rough natural fractures on particle transport remains poorly understood.
In this study, we constructed a 3D-printed rough fracture model to investigate the transport behavior of micro-particles within the rough fracture. Here, we develop a particle transport imaging system using silica micro-particles coated with fluorescence material, in conjunction with a Particle Image Velocimetry (PIV) system. We investigated the transport and settling behavior of fluorescent micro -particles in several rough fracture models under different fluid injection rates, and fracture roughness. The experimental results revealed that as the surface roughness of a fracture increases, the particles tends to settle more rapidly near the entrance of the fracture. This phenomenon substantially diminishes the lateral transport of the particle within the fracture, leading to a swift accumulation and consequent plugging at the entry of the fracture. Notably, even with a increased fluid injection rate, the rough fracture are not entirely obstructed by the clogging of particles. The overall findings will shed light on understanding clogging and deposition characteristics of particles in subsurface rough natural fractures.

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MS06-A / 369

Experimental and numerical studies of spontaneous imbibition in sandstones

Authors: Chaozhong Qin[1]; xin wang[None]

Co-author: Bo Guo [2]

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Spontaneous imbibition (SI) driven by the capillary force is pivotal to diverse earth science applications. To elucidate the interplay between capillary and viscous forces during spontaneous imbibition in porous media, the pore-network model proves to be an efficient tool. We initially verify our dynamic pore-network model against a series of water-air spontaneous imbibition experiments on three sandstones with distinct pore structures, which can be established under both constant and distributed contact angles. We then compare spontaneous imbibition with reduced viscosity ratios and quasi-static imbibition. However, we observe discrepancies in pore-filling events and the associated average transport properties under these two wettability conditions, leading to disparate imbibition rates and wetting saturation at lower viscosity ratios. Furthermore, when comparing spontaneous imbibition experimental data across a spectrum of nonwetting phase viscosities from the literature, we find superior model fitting with a constant contact angle. Although recent findings suggest that contact angles in pore spaces tend to follow a lognormal distribution, such a distribution may not be appropriate for the pore-network model with already simplified geometric pore characteristics. Our research also indicates that the correspondence in imbibition rate and wetting saturation against experiments at each viscosity ratio is the definitive validation criterion for the pore-network model of spontaneous imbibition.

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MS11 / 370

Microfluidic Visualization and Modeling of Polymer Induced End-Point Relative Permeability Damage

Authors: Shaken Kenzhekhanov[1]; Xiaolong Yin[2]

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After polymer injection, the end-point relative permeability of porous medium to other fluids often drops significantly and is not the same as that prior to polymer injection. To understand the hydrodynamic mechanism of this change, we conducted microfluidic experiments. We discovered that polymer solutions were mostly found in pores that are aligned with the direction of mean flow. At the end-points, to flow around the polymers, oil / water needed to use channels that are not aligned. Their flow pathways hence became more tortuous. To quantify the effect of pathway tortuosity, orientation distributions of fluids in the microfluidic porous medium were measured. They were then coarsened into four bins consisting of channels 0, 30, 60, and 90 degrees relative to the direction of mean flow. By treating the microfluidic porous medium as a superposition of two inter-penetrating honeycombs, we show that the observed distributions of fluids at the end-points could largely explain the changes in the end-point relative permeabilities, proving the tortuosity of the flow was indeed a significant contributor to end-point relative permeability damage.

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MS10 / 371

Gas Invasion Behaviors and Failure Patterns within Layered Porous Systems Investigated by X-ray CT

Author: Zhenqi Guo[1]

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Gas trapping and escaping in layered geological settings widely occur. We utilized an in-situ gas injection apparatus based on high-resolution micro-CT to investigate gas invasion behaviors and

deformation patterns of layered porous media systems. The system includes a reservoir and a cap layer with carefully controlled capillarity and permeability. Results show that all cases experience cycles of a pressure built up period and a sudden pressure release when a barrier, either capillarity or effective stress, is overcome. Drainage conditions significantly impact both the trapped gas volume and deformation patterns. Effective stress analyses show that dominant factors are capillarity Pc, *effective stress σ' and excess pore fluid pressure Δu, affected by gas injection rate, cap layer thickness and permeability. Five deformation patterns, capillary invasion, fracture opening, integral uplifting, local heaving and violent liquefaction are identified according to two dimensionless number χC/E = Pc/σ'* and $\chi P/E = \Delta u / \sigma'$.

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Poster / 372

Plugging rules, macro-micro matching relationship and EOR mechanism of elastic particle: A microfluidic study

Authors: Xin Chen[1]; Shun Liu[1]; Jianbin Liu[1]

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The transport of elastic particles (EP) in porous media occurs extensively in groundwater filtration, fluidized beds, and oil field development. However, the pore-throat migration rules and the macro- and micro-matching relationship between EP and porous media require further study. In this work, four mechanism models were designed to conduct microfluidic injectivity experiments. By analyzing the pore throat flow behavior of EPs, their migration and plugging rules can be clarified. The microscopic matching characteristics of EPs and pore throats are evaluated based on their entry and retention status in throats of different sizes. Meanwhile, comparing the results of our previous macroscopic matching experiments can achieve the unification of macroscopic and microscopic matching between EPs and pore throats. In addition, microfluidic oil displacement experiments can be carried out based on the reservoir model, and the enhanced oil recovery (EOR) mechanism can be elucidated. The results show that EPs exhibit a "Gather-Energized" transport mode in porous media: as the injection pressure increases, EPs accumulate in the pores, then gradually enter the throat, and finally migrate away from the model outlet. The "Gather-Energized" transport mode and elastic deformation performance of EPs determine that they have the characteristics of pore-throat matching and preferential plugging of large pore-throats. According to the change in the pressure difference between the end time of EP injection and subsequent water injection, it can be determined that the upper limit of the microscopic matching factor is 1.3-1.4, and the optimal matching factor range is 0.8-1.0. The macro and micro matching relationship between EP and pore throats is highly consistent. After water flooding, EP can increase oil recovery by 6.95% compared to polymer flooding.

The EOR mechanism mainly includes activating continuous remaining oil, increasing the injection-production pressure difference, and increasing the oil washing efficiency in the swept volume. The experimental results and conclusions of this work support the feasibility of using microfluidic experiments to replace complex core displacement experiments to evaluate the transport and matching characteristics of EPs.

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MS07 / **373**

A lattice Boltzmann based Darcy-Brinkman-Stokes method for micro-continuous two-phase flow

Author: Yang Liu[1]

Co-authors: JingSen Feng ; JingChun Min [1]

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The transport of immiscible two-phase in porous media involves many scientific and engineering fields, such as hydrogeology, reservoir development and electrochemical energy storage. This kind of flow phenomenon usually occurs in multiscale pores from micro to macro, making direct numerical simulations suffered from huge computational costs. Considering the demand for simultaneously mimicking both porous Darcy flow at micro-continuum scale and free Stokes flow at pore scale, the Darcy-Brinkman-Stokes (DBS) method based on volume-averaged Navier-Stokes (VANS) equation is established recently and it has made great contributions to study seepage flow and imbibition phenomenon in multiscale media [1,2].

Lattice Boltzmann method (LBM), as a mesoscopic numerical technology, has achieved great progress for complex multiphase flow in porous media. Thus, the combination model of LBM and DBS has significant advantages in multiscale flow simulation compared to traditional scheme (FVM, FDM), e.g., it is able to capture the discontinuity of velocity gradient at free-porous interface, and does not need data transmission and special boundary treatment between regions with different scales.

In our work, the improved color-gradient model [3] and a novel volume averaging technique [4] have been applied, which considers the streaming of effective densities, a forcing term for pressure correction and a source term for error correction for two-phase's density ratios. By adding a total force term in moment space including continuum surface force, drag forces induced by porous matrix, we have correctly recovered the multiple-relaxation-time (MRT) LB equation to VANS equation through Chapman-Enskog analysis, and thus a multiphase DBS-LBM model has been newly-established. Meanwhile, a capillary force containing a numerical interaction parameter is imple-

mented to mimic the apparent wettability in the spatially-distributed porosity field within micro-continuous porous areas. The standard validations have confirmed the accuracy and robustness of this new model, such as its flexible adjustability for interfacial tension and relatively low spurious currents, as well as it has good physical continuity at free-porous interface and stable numerical performance, especially in terms of simulating fluids with density/viscosity ratios. Besides, through the static droplet and dynamic capillary effect tests, the proposed interaction force has been demonstrated to be effective for trans-scale simulation of immiscible two-phase's transport and sorption behavior in multiscale pores.

In future study, developing this model to 3D is practical and straightforward, it will allow to simulate a larger multiscale structure at domain scale actually, where the parameters of micro-continuous porous areas can be obtained from grayscale CT scanning and experimental correlation. Moreover, a temporally varying porosity field can be incorporated by coupling the governing equations of solid components to simulate flow-structure problems in soft matter or particle clusters.

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1 Carrillo, F. J.; Bourg, I. C.; Soulaine, C. Multiphase flow modeling in multiscale porous media: An open-source micro-continuum approach. Journal of Computational Physics: X 2020, 8. DOI: 10.1016/j.jcpx.2020.100073. 2 Lu, S. F.; Wang, Y. X.; Ma, M. Y.; Xu, L. Water seepage characteristics in porous media with various conduits: Insights from a multi-scale Darcy-Brinkman-Stokes approach. Comput. Geotech. 2023, 157, 13, Article. DOI: 10.1016/j.compgeo.2023.105317. [3] Ba, Y.; Liu, H.; Li, Q.; Kang, Q.; Sun, J. Multiple-relaxation-time color-gradient lattice Boltzmann model for simulating two-phase flows with high density ratio. Physical Review E 2016, 94 (2). DOI: 10.1103/PhysRevE.94.023310. [4] Bukreev, F.; Simonis, S.; Kummerländer, A.; Jeßberger, J.; Krause, M. J. Consistent lattice Boltzmann methods for the volume averaged Navier–Stokes equations. J. Comput. Phys. 2023, 490. DOI: 10.1016/j.jcp.2023.112301.

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Poster / 375

The Mechanism and Quantification of Threshold Pressure for Oil Flow in Silica Nanochannel by Molecular Simulation

Authors: BingBing Liu[1]; Jie Zhong[1]; Youguo Yan[1]; Jun Zhang[1]

Co-author: Xiao Wang [1]

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

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Shale oil is an abundant unconventional resource in the world. However, due to the highly heterogeneous of shale reservoirs, the shale oil is difficult to flow in the porous media, resulting in the uncertainty efficiency of industrial exploration for shale oil. Threshold pressure gradient is the key property to characterize the mobility of shale oil. Usually, shale rock has abundance of pores in

nanometer, and the structure is more tight than other reservoirs. It is challenging to study threshold pressure gradient for shale oil by traditional theoretical and laboratory methods in low-permeability reservoirs. In view of this, our work will quantify the threshold pressure gradient and reveal the mechanism of threshold pressure for fluids flow at nanoscale by molecular simulation. In our work, the threshold pressure of oil flow in silica nanochannel was quantified firstly by "pressure - velocity"method. The "pressure-velocity"shows the oil flow would be divided into three stages, via vibrate stage, initial stage and flow stage, showing non-Darcy flow. After that, the size of silica nanopore with 2nm, 4nm, 6nm, 8nm and 10nm, was constructed to study the size effect of threshold pressure. The calculated threshold pressure indicates that the critical pressure for oil to flow in nanopores would exponential increased with the decrease of height. When the height of nanochannel increases to 10nm, the threshold pressure was very small. Also, the height of silica nanochannel would influence the fluids properties, such as density, viscosity, etc. Due to the decrease of nanochannel, the proportion of adsorbed oil molecules in nanochannel would increase, thus influencing the viscosity and critical pressure to flow. Meanwhile, with the decreased nanochannel, the interaction between shale oil and nanochannel would increase, and more pressure are needed to make the shale oil flow. There is a highly correlation between threshold pressure and interaction energy. Intrinsically the critical pressure of oil is the energy needed to disturb or force the adsorbed oil film flow in nanochannel. Furthermore, the threshold pressure for shale oil is also related with rock types, such as quartzite, carbonate and kaolinite, etc, especially for oil in very small nanochannel. Our work provides a new insight into the shale oil flow in porous media, which is meaning for exploration of shale oil resources.

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Poster / 376

Experimental and theoretical evidence for energy signal indicating flow regimes for two phase flow in porous media

Authors: Shuangmei Zou[None]; Dong Chen[1]; Congjiao Xie[1]

[1] *China University of Geosciences(Wuhan)*

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Many studies have been dedicated to examining flow regimes using two key parameters: viscous ratios and capillary numbers Ca. However, only a few studies have elucidated mechanisms that govern different flow regimes and how the work of displacement and surface aeras alter within porous media, as well as their influence on flow behavior is still unknown. In this study, we experimentally investigate the combined effect of wettability and flow rates on immiscible fluid-fluid displacement using high-resolution imaging in microfluidic flow cells with two different viscous ratios. We investigate morphology of oil cluster and displacement front and further calculate the relative change of energy conversion based on external work and surface energy. The morphology

of invasion patterns in brine-silicone is sharper than that in brine-decane displacement, with the indication of larger ratios of length and width for fingers. The signature of the transition between the three regimes manifests itself in the efficiency of conversion of the external work to surface energy. Efficiency of conversion decreases with the increase of contact angles. With the increase of Ca, Efficiency of conversion reduces greatly to approximately zero. In high M displacement, efficiency of conversion is consistently higher than that in low M displacement. The signature of the transition between the three regimes (viscous flow, capillary dominated flow and capillary -stable displacement flow regime) manifests itself in the fluctuations of the external work and surface energy. We propose that it is possible to determine the nature of multiphase-flow displacement from the energy signal.

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MS10 / 378

X-ray microtomography imaging of two-phase fluid flow in water-wet and mixed-wet Bentheimer sandstone

Authors: Shuangmei Zou[None]; Dong Chen[1]; Congjiao Xie[1]

[1] *China University of Geosciences(Wuhan)*

Corresponding Author: shuangmei.zou@outlook.com

X-ray microtomography (micro-CT) provides a nondestructive way for estimating rock properties such as relative permeability. Relative permeability is computed on the fluid distributions generated on three dimensional images of the pore structure of a rock. However, it is difficult to numerically reproduce actual fluid distributions at the pore scale, particularly for a mixed-wet rock. Recent advances in imaging technologies have made it possible to directly resolve a large field of view for arbitrary wetting conditions.
Herein, the objective of this study is to evaluate relative permeability computations on imaged fluid distributions under water-wet and mixed-wet conditions. By simultaneously injecting oil and brine on a Bentheimer sandstone before and after wettability alteration, imaged fluid distributions are obtained under steady state conditions. Then we determine in situ phase saturations and capillary pressures from interfacial curvature measurements along an entire core, thus achieving the assessment of the capillary pressure gradient and its influence on multiphase flow. We demonstrate how the pore-scale capillary pressure gradient affects multiphase flow and, in turn, the core-scale relative permeability measurements. Analysis of imaged fluid distributions and connectivity demonstrates that under mixed-wet conditions , increased dynamic connectivity and ganglion dynamics result in non-equilibrium effects at the fluid-fluid interface. These effects result in more energy dissipation during fractional flow in mixed-wet systems and thus lower effective permeability than water-wet rock at the same saturation.

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Poster / 379

Pore network modelling to study dynamic permeability evolution of hydrate-bearing sediments considering media deformation

Author: Mingqiang Chen[1]

Co-authors: Qingping Li [1]; Weixin Pang [2]; Qiang Fu [2]; Chaohui Lyu [3]; Yang Ge [2]; Huiyun Wen [2]; Bo Yang [2]; Xiaohan Zhang [1]

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Permeability is a key parameter determining fluid flow dynamics and production behavior of hydrate-bearing sediments. Figuring out the evolution of dynamic permeability during hydrate phase transition considering media deformation effect is of great significance for the safe and efficient development of hydrate-bearing deposits. In this work, an unstructured pore network with the combination of complex pore-throat morphology and anisotropy is firstly constructed based on the analysis of microscopic pore structures from the marine sediments in the South China Sea. After the validation, grain-coating hydrate is assigned to the pore bodies, connected throats and adjacent pore bodies from large to small elements in the network while considering media deformation effect. Based on the generated hydrate-bearing networks with different hydrate saturation, the dynamic permeability evolution law coupling media deformation effect is calculated. Furthermore, the effect of media deformation on the effective pore structures and dynamic permeability evolution during hydrate phase transition is analyzed in detail. Results show that the absolute permeability grows smaller at the same hydrate saturation due to the compaction of the effective pore body and throat radius caused by media deformation. However, the dynamic permeability decline rate turns slower with the increase of hydrate saturation since hydrate just needs to possess less pore bodies and throats to arrive at the same hydrate saturation when considering media deformation effect. Therefore, the difference of the dynamic permeability with and without considering media deformation becomes smaller at the same hydrate saturation. With an increase in effective stress, a decrease in elastic modulus, and a reduction in Poisson's ratio, the influence of media deformation on the effective pore structures in hydrate-bearing sediments intensifies, resulting in a greater decrease in the effective pore-throat radius and a larger reduction in the dynamic permeability at the same hydrate saturation. In addition, the number of hydrate occupied pore bodies and throats grows much smaller at the same increase degree of hydrate saturation as media deformation effect becomes more pronounced,

which results in much slower rate of dynamic permeability reduction and smaller difference of the permeability at different values of parameters relavant to media deformation.

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Poster / **382**

A Robust Vapor-liquid-liquid Equilibrium Calculation Algorithm Considering Capillary Pressure and Critical Shift in Nanopores

Authors: Binyao Xiao[1]; Hai Sun[1]; Dongyan Fan[1]; Lei Zhang[1]; Shuaishi Fu[1]; Jun Yao[1]

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Porous media contains a huge amount of nanopores, and the behavior of confined fluid phases in nanopores will be affected by significant interfacial effects between the fluids and the walls. A large number of publications have recently investigated the influence of interfacial effects on the phase behavior of confined fluids in nanopores. Many influences such as adsorption, critical shift, capillary pressure have been discussed. However, most of these studies have focused only on vapor-liquid equilibrium (VLE), and few attempts have been made to generalize these influences to vapor-liquid-liquid equilibrium (VLLE) in nanopores. In this work, a robust and efficient algorithm for the calculation of VLLE is proposed. The algorithm can simultaneously consider the influences of capillary pressure and critical shift on VLLE in nanopores. In order to be able to accurately and efficiently calculate each of the possible phases, the algorithm adjusts some of the steps in the conventional VLE calculation and improves the solution methodology.

The results of VLLE in this algorithm are obtained from three-phase flash calculations. It is well known that three-phase flash calculations are extremely dependent on initial guess and have poor convergence properties. In order to solve this problem, this work couples the successive substitution iteration with the Newton-Raphson iteration and builds a joint solver. The results show that this coupled joint solver not only improves the computational efficiency, but also enhances the stability of the flash calculations.

The robustness of the present algorithm is verified by several computational examples, and influences of capillary pressure and critical shift on VLLE in nanopores are investigated. In this work, mixtures of hydrocarbons with water and carbon dioxide were calculated and several possible fluid distribution scenarios were considered. The computational results show that both capillary pressure and critical shift can change the phase distribution of the confined fluid in nanopores.

1. The effect of capillary pressure on phase behavior is determined by the wettability between nanopores and the confined fluids. When the nanopores have a higher affinity for the vapor phase than the liquid phase, the generation of the bubble point will be advanced and the generation of the dew point will be lagged. If wettability is reversed, the effect of capillary pressure on phase behavior of the system is also reversed at the same time.
2. Critical shift affects the phase behavior of confined fluids more than capillary pressure for a certain range of pore sizes. However, the critical shift is independent of the wettability. Regardless of the pore size, the effect of critical shift on phase behavior has the same trend.
3. The effect of pore size on the behavior of confined fluids is nonlinear. In other words, there is an inflection point in the trend of pore size versus the phase behavior, and when the pore size is higher than this inflection point, the effect of capillary pressure or critical shift can be neglected when calculating the VLLE. Based on the findings of this work, we believe that this inflection point lies around 100 nm.

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MS03 / **383**

Relative Permeability Cyclic Hysteresis and its Application in Improving the History Matching Quality and Evaluating Deliverability Capacity in a Fractured Carbonate Gas Reservoir Storage Field

Author: Junchang SUN[1]

Co-authors: Chun LI [2]; Jieming WANG [2]; Lei SHI [2]; QingJie ZHANG [1]; Runya SHEN [1]; Ruotong CHEN [1]; Xiaohu GUO [1]

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The SF reservoir in China is a naturally fractured but low permeability carbonate gas reservoir with average porosity and permeability about 4.3% and 3.7mD, respectively. Macro- and micro-fracture as well as large vuggy pore all developed in the reservoir making it quite heterogeneous. This reservoir has been converted to underground gas storage (UGS) after 25 years depleted production with the initial gas-water contact (GWC) rise of nearly 200m. Gas injection commenced in 2014.
It has long been observed that history matching of UGS dynamics is much poor even for many

weak water-drive sandstone reservoirs in China. Naturally, simulation prediction will be unreliable. To accurately quantify the actual deliverability capacity of the more complex SF UGS, a series of 5 cycles gas/water successive drainage and imbibition relative permeability and high rate injection/withdrawal physical simulations under realistic reservoir conditions were performed to better understand UGS dynamics behavior in the fractured reservoir and improve history matching quality. Then, a dual porosity simulation model was constructed and modified to determine the actual capacity of the SF UGS.
The simulation model achieves a good match of the historical reservoir pressure and production of gas, oil and water during past production through modifications of local matrix and fracture permeability, aquifer strength and well Productivity Indices (PI). However, history matching of the three years UGS operations is significantly poor. In fact, laboratory tests indicate that gas-water relative permeability exhibits significant hysteresis in tight matrix and micro-fractured samples. Particularly, irreducible water and residual gas saturation steadily increase, respectively, 2.8% and 25% in the matrix samples after 5 cycles'successive drainage and imbibition process suggesting the effective pore volume will significantly decline in the thick transition zone. It was also found that nearly 18% of the gas-filled pore volume cannot be utilized during the high rate withdrawal while it was effective in the primary depletion. According to the above experiments, hysteresis was considered by cycle-dependent relative permeabilities and repeated model restart. Deterioration of the effective pore volume was implemented through introducing heterogeneous matrix-fracture interaction coefficients based on integrated studies of fractures distribution and heterogeneous permeability. A better well static pressure and water production were then obtained while keeping the good history matching of the previous depletion.
Simulation prediction suggests that the maximum working gas volume may slightly less than 1.2bcm previously designed using reservoir engineering method and the deliverability is about 12 million cubic meters per day. Pressure sink and water coning are the two key factors limiting the UGS performance. This study reveals that reservoir simulation combined with physical simulations can better understanding reservoir dynamics and then give a more accurate prediction.

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MS03 / **384**

Prior ensemble based on geomechanical proxy model for data assimilation in naturally fractured reservoirs

Authors: Michael Liem[1]; Giulia Conti[None]; Stephan Matthai[2]; Patrick Jenny[None]

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Fractures can facilitate or alter fluid flow and transport in subsurface reservoirs. Consequently, their accurate characterisation is crucial for various applications, including geothermal heat extraction and carbon sequestration. Yet, direct measurement of relevant fracture parameters is difficult. Access is limited to wells, leading to significant uncertainties, particularly in estimating fracture aperture and length –key factors influencing flow and transport. The application of indirect methods, including outcrop analogue studies, geophysical imaging, tracer tests and production logging, is vital to mitigate these limitations. It is particularly effective when combined with data assimilation techniques like ensemble Kalman filters.

This study uses a fracture pattern with more than 3500 individual fractures mapped on aerial photographs (Odling, 1997). We assume that the fracture geometry is known *a priori* and focus on fracture aperture as the uncertain parameter. The fractures are subjected to a constant far-field stresses, causing critically stressed ones to shear and dilate. We represent this behaviour with the empirical joint constitutive model of Barton & Bandis (Barton et al., 1985). However, the exact aperture values remain unknown, as they depend on uncertain model parameters like fracture roughness and rock properties. Our goal is to reduce these uncertainties using an ensemble smoother with multiple data assimilation (ES-MDA) (Emerick & Reynolds, 2013) that will be informed with synthetic flow and transport data. Particular attention is given to the influence of the prior ensemble on the performance of the data assimilation framework.

Calculating individual realisations of the prior ensemble with a geomechanical simulator can become prohibitively expensive, especially when a large ensemble size is required. A cheaper, purely stochastic approach on the other hand does not incorporate all geological knowledge. As a compromise between these two methods, we generate the prior ensemble based on the far-field stress approximation (FFSA), a proxy model which projects the far-field stresses onto the fracture planes and approximates shear displacement with linear elastic theory. The FFSA is computationally efficient as it does not rely on geomechanical simulations, while still incorporating geological knowledge to some degree.

Our results demonstrate that FFSA-based prior ensembles significantly outperform stochastic ones, leading to more accurate estimations of fracture aperture and an improved alignment with synthetic reference data. Further, the FFSA requires smaller ensemble sizes than the stochastic approaches as it models aperture more accurately. We expect that these results can be generalised to other ensemble-based DA methods, for example particle filters.

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Poster / 385

Inferring electrochemical performance and parameters of Li-ion batteries based on deep operator networks

Authors: Qiang Zheng[None]; Xiaoguang Yin[None]; Dongxiao Zhang[None]; Qiang Ye[None]

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Li-ion battery is a complex physicochemical system that generally takes observable current and terminal voltage as input and output, while leaving some unobservable quantities, e.g., Li-ion concentration, for serving as internal variables (states) of the system. On-line estimation for the unobservable states plays a key role in battery management system since they reflect battery safety and degradation conditions. Several kinds of models that map from current to voltage have been established for state estimation, such as accurate but inefficient physics-based models, and efficient but sometimes inaccurate equivalent circuit and black-box models. To realize accuracy and efficiency simultaneously in battery modeling, we propose to build a data-driven surrogate for a battery system while incorporating the underlying physics as constraints. In this work, we innovatively treat the functional mapping from current curve to terminal voltage as a composite of operators, which is approximated by the powerful deep operator network (DeepONet). Its learning capability is firstly verified through a predictive test for Li-ion concentration at two electrodes. In this experiment, the physics-informed DeepONet is found to be more robust than the purely data-driven DeepONet, especially in temporal extrapolation scenarios. A composite surrogate is then constructed for mapping current curve and solid diffusivity to terminal voltage with three operator networks, in which two parallel physics-informed DeepONets are firstly used to predict Li-ion concentration at two electrodes, and then based on their surface values, a DeepONet is built to give terminal voltage predictions. Since the surrogate is differentiable anywhere, it is endowed with the ability to learn from data directly, which was validated by using terminal voltage measurements to estimate input parameters. The proposed surrogate built upon operator networks possesses great potential to be applied in on-board scenarios, since it integrates efficiency and accuracy by incorporating underlying physics, and also leaves an interface for model refinement through a totally differentiable model structure.

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Poster / 386

Criss-Cross Physics-Informed Convolutional NeuraNetworks for Prediction of Fluid Flow in Porous Media with Spatial Heterogeneity

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Recent breakthroughs in deep neural networks have brought about transformative insights into the realms of physics, engineering, and scientific computing. Addressing the integration of neural networks with physical simulation remains a paramount research focus, where the physics-informed neural network (PINN) stands out as a widely adopted framework due to its versatility in constructing neural networks and exceptional generalization capabilities. However, challenges arise in enforcing flux continuity across boundaries between cells with varying physical properties, particularly in scenarios involving spatial heterogeneity. This work introduces a novel paradigm, the criss-cross physics-informed convolutional neural network (CC-PICNN) learning architecture, specifically designed to address the solution of parametric partial differential equations (PDEs) in the presence of spatial heterogeneity in physical properties. The central objective is to seamlessly enforce flux continuity while imbuing convolutional neural networks (CNNs) with meaningful physical interpretations. A key innovation is the introduction of a predefined 2D convolutional layer to accurately express transmissibility between adjacent cells. To assess the effectiveness of the proposed CC-PICNN method, a comprehensive evaluation is undertaken using petroleum reservoir problems characterized by spatial heterogeneity. The performance of CC-PICNN is benchmarked against the state-of-the-art PINN through meticulous numerical analyses, revealing the superior efficacy of the proposed method. This research not only contributes to advancing our understanding of addressing spatially heterogeneous scientific challenges but also provides a more robust and effective solution compared to existing approaches, particularly PINN. The proposed CC-PICNN framework holds promise for applications demanding accurate modeling of physical properties in diverse scientific domains.

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Poster / 387

Physical characteristics analysis of Carboniferous-Jurassic reservoir in the piedmont southwest Tarim Basin

Authors: Boyu Wang[1]; Jie Yin[1]; Lin Ye[1]; Zhenqi Wang[1]

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The southwest Tarim Depression is an important exploration area in the Tarim Basin. In recent years, an major breakthrough has been made in the substantial increase of exploration reserves, indicating that this area has great exploration and research potential. Collect the Carboniferous-Jurassic reservoir samples from five profiles in the front of Kunlun Mountain in the southwest of Tarim were, combined with the casting thin sections and scanning electron microscopy to analyze their physical properties. The results show that: The sedimentary environment of the Carboniferous reservoir in the study area is mainly carbonate platform, the Permian reservoir mainly develops delta distributary channel, underwater distributary channel and fluvial sand conglomerate, and the Jurassic

reservoir is the sandstone reservoir of delta and lake deposits. On the whole, the average porosity of the sandstone reservoir is about 2.24%, the highest permeability is only 3.34×10-3μm2, and the average is about 1.19×10-3μm2. The porosity and permeability are low, and the reservoir physical properties are poor. The reservoir space is the dissolving pore - intergranular pore - dissolving pore and fissure-pore. The porosity and permeability of carbonate reservoirs are relatively good, with an average porosity of about 1.54% and an average permeability of about 8.93×10-3μm2, but it is still dominated by Class II and Class III reservoirs, and the reservoir space is the assemblage of pore - fracture, and fracture.

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MS09 / **388**

The numerical simulation of two-phase flow in multi-mineral shale digital rock cores

Authors: Guangyuan wei[1]; Hai Sun[1]; Lei Zhang[1]; Dongyan Fan[1]; Shuaishi Fu[1]; Jun Yao[1]; Yongfei Yang[1]; Junjie Zhong[1]

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Shale oil and gas resources are widely distributed and have abundant reserves in China, with broad development prospects and potential. Due to the inherent characteristics of shale oil, such as the large number of nanometer-sized pores with complex pore structures, significant fluid-wall effects, complex mineral compositions, abundant organic matter, and complex and diverse wettability, the flow law of multiphase flow under shale reservoir conditions differs significantly from conventional reservoirs. Therefore, it is essential to characterize the flow of multiphase flow under shale pore scales, considering TOC content, complex wettability, and adsorption conditions. In this work, a new method for simulating the pore scale of shale oil-water two-phase flow based on mixed multi-mineral phase digital cores is proposed. This method is based on identifying the pore wall surfaces of each mineral and considering the corresponding adsorption and wettability conditions. Firstly, the multi-mineral phase shale digital core is reconstructed from the two-dimensional scanning electron microscope image of the shale sample, and the pore space of the corresponding minerals is divided by grids. Secondly, based on the Navier-Stokes equation, considering the TOC content, complex wettability conditions, and adsorption layer, the VOF method is used to simulate the shale oil-water two-phase flow process at the pore scale. Finally, the influence of TOC content, complex wettability, and adsorption on the shale oil-water two-phase flow is analyzed. The results have shown that the effects of TOC content, complex wettability, and adsorption on shale oil-water two-phase flow cannot be ignored. As the TOC content increases, the contact area between the organic pore walls and oil and water also expands. The flow of the water phase is hindered by the oil-wet organic pore walls, which significantly reduces the movable degree of oil. The movable degree of oil is also

influenced by the organic matter distribution. In addition, the change in wettability of shale pore walls can also affect the flow of oil and water phases in shale. With the stronger oil-wetness of shale pore walls, especially organic pore walls, the movable degree of oil decreases. Due to the narrow pore radius and strong fluid-wall interaction, the adsorption phenomenon is significant, causing oil to remain on the pore surface, thus, greatly reducing the movable degree of oil. Our findings are critical for enhancing the efficiency of shale oil recovery, carbon dioxide geological sequestration, and other related areas.

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Pollution Remediation and Control of Karst Underground River —A Case Study of the Pingqiao Underground River System, Zunyi, China

Author: changsong zhou[None]

Co-authors: shiyou yi ; shengzhang zou

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Based on years of investigation, assessment, and practical pollution control, this study establishes a model suitable for pollution remediation and control in karst underground rivers—the Three Source Model. This model primarily includes dual-source investigation, source-to-sink tracking, and source control. Taking the Pingqiao Underground River system in Zunyi City, with a pollution history of nearly 20 years, as an example, the Three Source Model is applied to the practical pollution remediation and control of this underground river.

The results of the dual-source investigation indicate that various types of water points are distributed in the study area, mainly boreholes, karst springs, and underground river outlets. The characteristic pollutants are primarily NH4+, NO3-, SO42-, Mn2+, and Se2+. Additionally, various pollution source points are distributed, mainly industrial waste disposal sites, predominantly located downstream in the Pingqiao Industrial Park area. The characteristic pollutants are also primarily NH4+, NO3-, SO42-, Mn2+, and Se2+.

Results from source-to-sink tracking reveal three groundwater pollution channels within the scope of the underground river system: 1) PQE019 (stilling tunnel) - PQG025 (skylight) - PQS009 (underground river outlet) pollution channel; 2) 2# waste residue disposal site flood discharge shaft - CK8 (borehole) - J02 (monitoring well) - CK6, CK11 (borehole) - JC04 (monitoring well), ZK2 (borehole) - PQG025 (skylight) - PQS009 (underground river outlet) pollution channel; 3) 1# waste disposal site - PQG025 (skylight) - PQS009 (underground river outlet) pollution channel. These pollution channels are distributed between the outlet of the underground river and the Z1（1#、2#）waste disposal site in Pingqiao Industrial Park.

Results from source control indicate that after repairing the upstream section of the polluted channel from the flood discharge shaft of the 2# waste disposal site to the outlet of the underground

river through curtain engineering, the groundwater level upstream of the curtain steadily increased (from 815.68m to 823.35m). There was no significant change in the groundwater level downstream of the curtain. During the non-pumping stage of the pumping wells PWZK1 and PWZK2, the NH4+ content at the outlet of the underground river was 76-143.6mg/L, the Mn2+ content was 14.206-21.31mg/L, and the outlet flow rate was 5.0-295.349L/s. However, During the intermittent pumping stage of pumping wells PWZK1 and PWZK2, the concentrations of NH4+ and Mn2+ at the outlet of the underground river show a downward trend during the pumping period, while the concentrations show a significant upward trend during the cessation of pumping. During the continuous pumping stage of pumping wells PWZK1 and PWZK2, the concentrations of NH4+ and Mn2+ at the outlet of the underground river remain relatively low, with NH4+ content generally ranging from 14.4 to 58.6mg/L and Mn2+ content generally ranging from 2.38 to 6.39mg/L. The concentrations of NH4+ and Mn2+ decrease by 66% -78% compared to the non-pumping stage. The calculation results of reducing pollutant emissions in the treatment project show that the underground river outlet can reduce wastewater emissions by 47244m3/a, with a minimum reduction of 16250kg/a for NH4+ and 10960kg/a for Mn2+.

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MS07 / 391

Multilevel Monte Carlo Method for Simulation of Propagation of Uncertainties in Fractured Porous Media

Author: Dmitry Logashenko[1]

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Simulation of salinization of coastal aquifers plays an important role in prediction of availability of pure water resources. In these geological formations, fractures introduce strong heterogeneities and their influence on the groundwater flow and the transport of the salt is significantly (cf. 1). However uncertain variations in hydrogeological parameters such as porosity, permeability, fracture aperture etc. may essentially reduce accuracy of the prediction of the transport phenomena. In this talk, we present an application of the multilevel Monte Carlo method for estimation of propagation of the uncertainty from the parameters of the fractured porous medium to the solution in the subsurface density-driven flow model represented by a system of non-linear PDEs. This research is a continuation of our recent work on the uncertainty quantification for this type of models (cf. e.g. 2). We test this approach on a model problem with the random porosity field, recharge and fracture aperture that represent the limited knowledge of the data. Parallelization is applied to the Monte Carlo method. We present results of numerical experiments on the supercomputer Shaheen II.

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2 A. Litvinenko, D. Logashenko, R. Tempone, E. Vasilyeva, G. Wittum, Uncertainty Quantification in Coastal Aquifers Using the Multilevel Monte Carlo Method, PAMM, 2023. DOI: 10.1002/pamm.202300005

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Poster / 392

Application of gel particles in the regulation of oil-water permeability curve

Authors: Quanling Qin[1]; Jian Hou[1]; Kang Zhou[2]

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In chemical oil drive technology, injecting polymers and surfactants is considered an effective method for adjusting the permeability of reservoir rocks, thereby influencing the flow characteristics of oil and water phases. While the effects of polymers and surfactants on the relative permeability of oil and water have been extensively studied, the impact of gel particles on the oil-water phase permeability curve remains under-researched. In this study, we intend to conduct a series of oil-water two-phase flow experiments under laboratory conditions, aiming to explore how different types, particle sizes, and concentrations of gel particles affect the phase permeability curves. Through these experiments, we aim to achieve an in-depth understanding of how the physicochemical properties of gel particles specifically influence the oil-water two-phase flow characteristics. We anticipate that the concentration and particle size of the gel particles will be key factors in determining the shape and location of the phase penetration curves. Additionally, numerical simulations will be utilized to model the reservoir-scale flow characteristics of gel particles and their potential impact on the oil-water phase infiltration curves, aiming to attain a more comprehensive understanding of how gel particles can enhance oil-water phase infiltration performance. The findings of this study hold significant importance in optimizing oilfield displacement. By rationally selecting the type, concentration, and particle size of gel particles, an effective enhancement in oilfield recovery is expected, thereby offering new perspectives for oilfield development.

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Experimental investigation of interplay between transverse mixing and reaction for pH reaction in porous media

Authors: Adi Biran[1]; yaniv edery[2]

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pH-induced reactive transport in porous environments is a critical factor in Earth sciences, influencing a range of natural and anthropogenic processes such as mineral dissolution/precipitation, adsorption/desorption, microbial reactions, and redox transformations. These processes, pivotal in carbon capture and storage (CCS) applications to groundwater remediation, are determined by pH transport and biogeochemical reactions. However, the uncertainty in these macroscopic processes' stems from pore-scale heterogeneities and Peclet. While practical for field-scale applications, traditional macroscopic models often fail to accurately predict experimental and field results in reactive systems due to their inability to capture the intricate details of pore-scale transport and reaction.
This study investigates the interplay between transverse mixing and pH-driven reaction in porous media. It focuses on how porous structure and flow rate affect mixing and chemical reaction dynamics. Utilizing confocal microscopy, the research visualizes fluorescently labeled fluids, revealing variations in mixing patterns from diffusive in homogenous to shear-driven in heterogeneous media. However, pH-driven reactions show a different pattern, with a faster reaction rate, suggesting quicker pH equilibration between co-flowing fluids than predicted by transverse dispersion or diffusion. The study highlights the unique characteristics of proton transfer in water, which significantly influences reactive transport in porous media.

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MS03 / **394**

Homogenization of flow and solute transport in fractured media using hybrid upscaling method

Authors: Bowen Ling[1]; Yujie Wang[2]

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Abstract:

Fractured media can be found in various natural and engineering systems, and the presence of fractures and fracture networks has a significant impact on the flow and transport processes at different scales. However, the complex nature of fractures poses challenges for theoretical modeling and numerical analysis. In this study, we propose a new hybrid upscaling workflow that combines analytical solutions at the continuum scale with fracture network methods. This method aims to preserve the connectivity of the fracture network and account for the interactions between fractures and the surrounding matrix. To validate the effectiveness of the new method, we compared its results with pore-scale simulations. Additionally, we investigated the influence of factors such as permeability, fracture aperture, porosity, and pore structure on the media. Through rigorous accuracy analysis and parameter studies, we assessed the applicability and computational efficiency of the proposed upscaling method.

Key words: fracture network; flow and transport in fractured media; Hybrid upscaling method

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MS01 / **395**

Production dynamic prediction and injection production efficiency optimization simulation of depleted gas storage reservoirs

Author: Hao Feng[1]

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In the construction and operation of depleted gas reservoirs underground gas storage, the block pressure, effective storage capacity, injection and production capacity, and operating cycle are key issues that reflect the storage efficiency of gas storage facilities. This article is based on the geological and structural characteristics, geometric characteristics, and physical properties of a sandstone reservoir in a gas storage facility in Liaohe Oilfield. Combining logging data and production performance data, a joint back analysis method for storage performance parameters is proposed to establish a three-dimensional fine geological model that can comprehensively reflect the construction and operation characteristics of the gas storage. By fitting the production dynamic history, the block pressure and single well pressure variation characteristics were simulated, and the model can effectively invert the changes in block pressure and single well pressure of the reservoir during 30 years of oil and gas production and 9 years of operation as a gas storage facility. On this basis, the model was used to predict the production dynamic operation of the gas storage, simulate the effects of injection and production rate, well network deployment, and injection and production cycle on the block operating pressure and oil-gas-water interface migration characteristics, and the upper limit of the effective storage capacity of the gas storage was predicted. This research achievement has guiding significance for exploring the operating rules of gas storage, analyzing storage capacity parameters and operational dynamics, and formulating reasonable working systems for injection and production wells.

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Poster / **396**

Direct numerical simulation of the two-phase flow in a pore network and comparative analysis with drainage/imbibition tests on glass micromodels

Author: Nadia Bali[1]

Co-authors: Anastasia Strekla [2]; Christina Ntente [1]; Maria Theodoropoulou [1]; Jeff Gostick [3]; Christos Tsakiroglou [1]

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The experimental and numerical study of drainage and primary/secondary imbibition cycles of immiscible displacement are crucial for several practical applications such as the spreading of oil pollutants in soils and groundwater, the in-situ remediation by water flushing, and the enhanced oil

recovery (EOR) from reservoir rocks. In order to simulate two-phase flow in pore networks, by now, most attention has been paid on mechanistic pore network models (PNM) and Lattice Boltzman (LB) approaches. The prediction of the two-phase flow pattern with direct numerical simulation, though computationally cumbersome, is a challenge. To address such a challenge, several numerical approaches are available, like the level set method, where issues such as maintaining a zero net mass balance equation remain unresolved 1. In this context, a phase field approach 2 is used to model the immiscible displacement of two fluids within the pore network of a specific micromodel [3]. Central to this approach is the Cahn-Hilliard fourth-order partial differential equation, governing the dynamics of the chemical potential (G) and mobility (γ). These parameters are intrinsically linked to key physical factors such as interphase thickness (ε), capillary width, mixing energy (λ), and surface tension coefficient (σ), Eqs. (1)-(3)

(1)$\partial\varphi/\partial t+u\nabla\varphi=\nabla\gamma\nabla G$

(2)$G=-\lambda[\nabla^2\ \varphi+(\varphi(\varphi^2-1))/\varepsilon^2\ ]$

(3)$\sigma=(2\sqrt{2})/3\ \lambda/\varepsilon$

The pore network is reconstructed from an actual glass-etched micromodel, for which extensive experimental data are available for validation and comparative analysis. This reconstruction is based on the software developed by the OpenPNM team [4], and the resulting geometry is then integrated into the Comsol Multiphysics® commercial software for simulation. In the numerical model, the Cahn-Hilliard equation is utilized to predict phase distribution under varying values of viscosity ratio, κ (=μinjected/μdisplaced), Reynolds number, and Capillary number. For mesh generation within the micromodel, approximately 2 million are used for network width W=10.1 cm and length L=15.3 cm. Depending on the initial conditions set, each simulation in this time-dependent model runs for a duration of 7 to 12 hrs.

To evaluate the model validation, the numerical results are compared with corresponding experiments of drainage/imbibition cycles, performed under varying fluid properties and flow conditions [5]. Special attention is paid on the potential to predict numerically the visualized flow pattern and the measured transient response of the pressure drop, when the oil phase in drainage or the aqueous phase in secondary imbibition are non-Newtonian shear-thinning fluids, by accounting for the actual fluid rheology. During the drainage stage, there is a notable agreement between the experiment and the numerical model. Discrepancies, minor in nature and within a 20% deviation, can be attributed to the idealized structure inherent in numerical simulations. Additionally, the consistency between 3D and 2D model outcomes suggests that a two-dimensional representation adequately captures the complexities of the problem without significant loss of information.

Acknowledgments

This work was performed under Grant Agreement 101037509 —SCENARIOS —H2020-LC-GD-2020 / H2020-LC-GD-2020-3 (project title: “Strategies for health protection, pollution Control and Elimination of Next generAtion RefractIve Organic chemicals from the Soil, vadose zone and water”-acronym “SCENARIOS”) supported by the European Commission.

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MS06-A / 397

Spatial characterization of wetting in porous media using local lattice-Boltzmann simulations

Author: Hamidreza erfaniGahrooei[1]

Co-authors: Reza Haghanihasanabadi [2]; James McClure [3]; Edo Boek [4]; Carl Fredrik Berg [5]

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Wettability is one of the critical parameters affecting multiphase flow in porous media. The wettability is determined by the affinity of fluids to the rock surface, which varies due to factors such as mineral heterogeneity, roughness, ageing, pore-space geometry, etc. It is well known that wettability varies spatially in natural rocks, it is still generally considered a constant parameter in pore-scale simulation studies. The accuracy of pore-scale simulation of multiphase flow in porous media is undermined by such inadequate wettability models.

The advent of in-situ visualization techniques, e.g., X-ray imaging and microtomography, enables us to characterize the spatial distribution of wetting more accurately. There are several approaches for such characterization. Most include the construction of a meshed surface of the interface surfaces in a segmented X-ray image and are known to have significant errors arising from insufficient resolution and surface-smoothing algorithms.

This work presents a novel approach for spatial determination of wetting properties using local lattice-Boltzmann simulations. The scheme is computationally efficient as the segmented X-ray image is divided into subdomains before conducting the lattice-Boltzmann simulations, enabling fast simulations. To test the proposed method, it was applied to two synthetic cases with known wettability and three datasets of imaged fluid distributions. The wettability map was obtained for all samples using local lattice-Boltzmann calculations on trapped ganglia and optimization on surface affinity parameters. The results were quantitatively compared with a previously developed geometrical contact angle determination method.

The two synthetic cases were used to validate the results of the developed workflow, as well as to compare the wettability results with the geometrical analysis method. It is shown that the developed workflow accurately characterizes the wetting state in the synthetic porous media with an acceptable uncertainty, and is better to capture extreme wetting conditions. For the three datasets of imaged fluid distributions, our results show that the obtained contact angle distributions are consistent with the geometrical method. However, the obtained contact angle distributions tend to have a narrower span and are considered more realistic compared to the geometrical method.

Finally, our results show the potential of the proposed scheme to efficiently obtain wettability maps of porous media using X-ray images of multiphase fluid distributions. The developed workflow can help for more accurate characterization of the wettability map in the porous media using limited experimental data, and hence more accurate digital rock analysis of multiphase flow in porous media.

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Poster / 399

Numerical simulation for the reactive multiphase flow in porous media during the Carbon Capture and Storage process

Author: Wenxin Yang[None]

Co-authors: Hai Sun ; Lei Zhang ; Dongyan Fan ; Shuaishi Fu ; Junjie Zhong ; Jun Yao

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In recent years, the extensive using of fossil fuels has led to a substantial release of greenhouse gases, resulting in a pronounced warming trend in the Earth's climate. To mitigate the process of global climate warming, Carbon Capture, Utilization, and Storage (CCUS) projects have gained prominence, with the efficient sequestration of CO2 into geological formations becoming a focal concern. In the process of CO2 sequestration, the permeation behavior of CO2 in water crucially determines its storage capacity and rate. On the one hand, the dissolution of CO2 in water increases the storage capacity. On the other hand, some rocks in the formation, such as glauberite, will dissolve under the combined action of carbon dioxide and water, thereby increasing the storage space of carbon dioxide. To comprehensively investigate the various influencing mechanisms in the CO2 sequestration process, pore-scale simulations offer an effective approach, allowing for a microscopic examination of mechanisms and a systematic analysis of influencing factors to further guide the sequestration of CO2. The lattice Boltzmann method, as a mesoscale approach, efficiently facilitates multiphase and multiscale coupling, enabling the treatment of complex solid-liquid/gas-solid boundary conditions. Thus, in this study, the lattice Boltzmann method was adopted for research purposes.
In this study, a new LB model was built to consider the effect of both CO2 dissolution in water and salt dissolution mechanisms on the CO2 storage process. What's more, the CST-LB model was adopted to describe the interfacial mass transfer, and the VOP method was used to update the structure of porous media. The impacts of factors such as wettability, salt concentration, and porosity on the CO2 sequestration process were comprehensively explored. The results indicate that, during the displacement and dissolution processes of CO2 in the aqueous phase, an increase in CO2 concentration in water leads to the gradual dissolution of some soluble salts in the solid phase. But there are some risks. While this expands the storage space for CO2, the dissolution of soluble salts results in the phenomenon of breakthrough points between CO2 and water, forming preferential channels that cause a substantial outflow of CO2. Additionally, when the wettability angle of the rock phase is greater, after CO2 displacement, some water remains in the porous medium, reducing the CO2 storage space and consequently diminishing sequestration capacity. This study provides crucial guidance for the sequestration of CO2.

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MS12 / **400**

Evaluation of Relative Diffusivity of Hydrogen-Methane System for Underground Hydrogen Storage in a Depleted Gas Reservoir Using a Novel Pore-Scale Reactive Transport Model

Author: Qiuyue Zhang[None]

Co-authors: Renyi Cao ; Zhihao Jia

Corresponding Author: zqy13653124701@163.com

The depleted gas reservoir is considered as one of attractive ways for underground hydrogen storage (UHS). However, due to the chemical reaction during UHS, the diffusion coefficient of the H2-CH4 binary system is more difficult to evaluate. The objective of this paper is to establish a novel pore network model merging H2 reactive transport to evaluate the relative diffusivity of the H2-CH4 system for UHS in depleted gas reservoirs.

Firstly, a stochastic pore network model was constructed based on the pore-throat diameter distribution of a depleted gas reservoir. Then, the concentration and rate functions were defined in the pore network model, in which the diffusion transport through porous media was expressed by the Fick's law. And a power-law chemical reaction equation for H2-rock was added as the source term. Finally, the curve of the relative diffusion coefficient vs. hydrogen concentration of the H2-CH4 binary system was obtained by solving the governing equations, which could be used to determine the impacts of diffusion during UHS in depleted gas reservoirs.

The results show that the diffusion coefficient of the H2-CH4 system is related to H2 concentration, porosity, pressure, etc. The H2 diffusion coefficient is proportional to H2 concentration and pore-throat size but inversely proportional to pressure. The diffusion coefficient under low pressure is about 20 times that under high pressure. Under the temperature of 40℃ and the porosity of 0.247, the effective diffusion coefficient decreases from 2.4×10-7m2/s to 6.03×10-8m2/s when the pressure increases from 5MPa to 20MPa. Under the temperature of 40 ℃ and the pressure of 10MPa, the effective diffusion coefficient increases from 3.7×10-8m2/s to 1.21×10-7m2/s when the porosity increases from 0.2 to 0.32. Furthermore, under the temperature of 40℃, the porosity of 0.247 and the pressure of 10MPa, the H2 effective diffusion coefficient is about 5×10-9m2/s when the H2 concentration is 0.4, while the effective diffusion coefficient increases to 4×10-8m2/s when the H2 concentration is 0.6. In addition, considering the CH4 creation by the chemical reaction of H2, the H2 effective diffusion coefficient decreased due to the decreasing of H2 concentration and the increasing of CH4 concentration.

A novel pore network model merging H2 reactive transport was proposed in this paper to evaluate the relative diffusion coefficient of the H2-CH4 system during UHS in depleted gas reservoirs. The methodology could provide a reference for UHS in depleted gas reservoirs.

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401

The distribution characteristics of hydrocarbons in nanopores

Author: yifan li[1]

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Corresponding Author: 469106327@qq.com

Shale rocks are associated with nanopores as small as 2 to 10 nanometers. Within nanopores, the heterogeneous distribution of fluid molecules is caused by the pore wall-fluid interactions and the fluid-fluid interactions, which leads to the alteration of fluid densities compared to bulk conditions. As we know, pure fluids can exhibit as gas, liquid, or supercritical phases under bulk conditions. Our aim is to understand whether the phases in nanopores remian as the same as the phase in the bulk condition. In this study, the density variation of fluids in nanopores was investigated using molecular dynamics simulation (MDs). Results show that bulk fluids in the liquid phases could act as the gas-like phases in nanopores, thus leading to over-estimation of hydrocarbons in place in shale reservoirs. The findings in this paper provide deep insights into the distribution of hydrocarbons in nanopores from the perspective of nanoscale, and recommend a new method for HIP calculations.

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MS20 / **402**

Reconstruction of Multiscale Structures of Cerebral Vasculature

Author: Yuedi Wang[None]

Co-authors: Han Xiao [1]; Moran Wang [2]; Yang Liu

[1] *Tsinghua univeristy*

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The cerebral vasculature plays a vital role in nutrients delivery and metabolic waste removal in the brain, yet in which transport mechanisms are not fully understood. Numerical simulation is an effective approach for analyzing transport in the cerebral vasculature, depending on accurate acquisition of the cerebrovascular structure. However, the complex cerebrovascular structure poses a serious challenge for reconstruction of the entire vasculature.
Traditional methods for the reconstruction of cerebral vasculature include medical imaging and computational generation. Medical imaging relies on the scanning technology (such as DSA 1 and MRA 2). Despite its effectiveness in clinical research, it's limited by their inability to capture small vessels in vivo due to resolution constraints. Alternatively, computational generation including simulated annealing algorithm [3], can overcome resolution limitations but often fall short in providing structures morphologically compatible with the real cerebrovascular structure.
In this study, we present a novel method for reconstructing the multiscale cerebral vascular system, which integrates anatomical findings with medical imaging. The proposed model merges macrovasculature derived from medical imaging which reflects real morphology, with microvasculature from random generation which could reach the resolution of capillary network. This integration allows a more accurate representation of the entire cerebral vasculature. Consequently, the flow simulations based on this model are in good agreement with medical experiments. This model provides an effective tool for simulating and understanding transport in the cerebral vasculature.

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1 Frisken, S., Haouchine, N., Du, R., & Golby, A. J. Computerized Medical Imaging and Graphics (2022). 2 Duvernoy, H. M., Delon, S., & Vannson, J. L. Brain Research Bulletin (1981). [3] Keelan, J., Chung, E. M. L., & Hague, J. P. Physics in Medicine & Biology (2019).

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MS15 / 405

Stable Diffusion in Digital Rock Analysis: Applications, Challenges, and Future Prospects

Authors: Yutian Ma[1]; Qinzhuo Liao[2]; Zhengting Yan[2]; Shaohua You[2]; Gensheng Li[2]

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Digital rock analysis has shown promise in visualizing geological microstructures and elucidating transport mechanisms in subsurface rocks, particularly in unconventional reservoirs such as tight sandstone and shale. Accurate image reconstruction techniques, which provide valuable insights into the pore network, grain distribution and connectivity, are essential to capture the intricate features and heterogeneity present in digital rock samples.

Stable diffusion (SD), a new hotspot in the field of artificial intelligence-generated content (AIGC), holds promising potential for the production of high-quality digital rock images. The SD is a deep learning model based on diffusion techniques, and has revolutionized the field of computer vision by generating highly realistic images from textual prompts, since its first release in 2022. While it is already being used in fields such as illustration, game design and electronic-commerce, its application in the digital core field is still in its early stages.

In this study, we examine the primary applications of SD in the field of digital rock analysis. Specifically, we explore its potential in enhancing image resolution, improving image quality through denoising and deblurring techniques, segmenting images into multiple regions, filling in missing sections, extending images in any direction using outpainting, and reconstructing 3D digital rocks based 2D images. Furthermore, this research highlights certain limitations of existing pre-trained models such as WebUI, Midjourney, and DALL-E. These limitations come from the fact that their databases do not encompass digital rock images obtained from scanning electron microscopes (SEM) or computed tomography (CT). Therefore, it is imperative to fine-tune the existing models or develop new ones specifically tailored to the realm of digital rock analysis, which deserves further attention and investigation.

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MS03 / **406**

A Darcy-Brinkman-Stokes Approach to Modeling Microbially Induced Calcium Carbonate Precipitation in Porous and Fractured Media

Authors: Xueying Li[None]; Xiaofan Yang[1]

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Corresponding Authors: xfyang@bnu.edu.cn, lixueying@mail.bnu.edu.cn

Microbially induced calcium carbonate precipitation (MICP) is an eco-friendly solution in geotechnical engineering, particularly for applications in bioremediation and CO_2 sequestration. Mathematical models have been developed to describe coupled biochemical processes in geological media.

However, there is a lack of numerical methods capable of modeling MICP directly from a single set of equations, which poses challenges on practical engineering applications. In this paper, we developed a pore-scale numerical solver, MICPFOAM, using a unified framework based on the Darcy-Brinkman-Stokes equation for simulating MICP in both porous and fractured media. The solver is implemented based on the OpenFOAM environment. We then validated our model in two systems, i.e., a flow system and a reaction system. Results demonstrated that MICP was significantly slower in fractured media than in porous media because of the preferential flow. In the reaction-diffusion system, strong diffusion ($D = 10^{-6}$) drove MICP far from equilibrium, while fast precipitation ($K_p = 10^{-2}$) combined with low ureolysis ($K_u = 10^{-5}$) promoted MICP to reach equilibrium. The initial biomass distribution is able to determine the occurrence of MICP, while biomass density only affects the amount of $CaCO_3$ after reaching equilibrium. Our model facilitates the coupling of biogeochemical properties in typical porous and fractured media, offering an applicable framework to model versatile processes and providing optimal conditions for potential MICP applications.

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409

Pore structure variations of felsic shale oil reservoirs to injected fluids: with implications to fracturing

Authors: Demiao Shang[1]; Xiaofeng ZHOU[1]; Jianguang WEI[1]; Fahimeh Hadavimoghaddam[1]

[1] *Northeast Petroleum University*

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In this paper, a felsic shale oil reservoir in China is chosen as the topic of research. The objective of this study is to understand how the pore structure of the formation would get altered as a result of injected fluid injections since the formation undergoes fracturing.
To achieve the goals of this study, a combination of laboratory methods were employed. A few samples are retrieved from several depths and locations of the formation for a better representation. CT scanning, electron microscopy, MICP and NMR tests were carried out to determine the best technical means of reservoir pore structure characterization. Samples were examined before exposure to injected solutions and following the exposure in reservoir conditions to delineate pore structure sensitivity and alterations.
By comparing the results of various pore structure characterization methods, a detailed understanding of pore structure variations with different perspectives was achieved. For instance, CT scanning visually delineated pore structure alterations through 3D images, and when combined with electron microscopy (FE-SEM) with higher resolution more detailed changes were observed. Furthermore, NMR method was found the most ideal approach to characterize the pore structure of shale oil reservoirs because of its wide range of pore accessibility since it is hydrogen sensitive, relatively low cost,

and being non-destruction to the samples which requires least sample preparation. The results of core immersion experiments showed that strong acid solution (15%HCL+3%HF) should have a moderate to strong improvement impact on the pore structure of felsic shale oil reservoir in the target block, while strong alkali solution (pH=13 NaOH) might damage the pore structures, and finally slippery water (neutral) will have a weak improvement of the samples'pore structure.
Considering the importance of fracturing to enhance production from shale plays around the globe, results from this study provide insights to the best approach in terms of the most suitable solution to inject as well as alterations that should be expected as the result of injection for optimum results in the field.

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Poster / 411

Numerical study on the enhanced oil recovery by CO2 injection and CO2 storage in shale oil formations

Authors: Rupeng Zhang[1]; Hai Sun[1]; Xinyi Zhao[1]; Dongyan Fan[1]; Lei Zhang[1]; Jun Yao[1]

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

Corresponding Authors: z22020047@s.upc.edu.cn, sunhai@upc.edu.cn, zxyzgsydx@outlook.com, zhlei84@163.com, fandongyan2010@126.com, yaojunhdpu@126.com

A larger part of oil in shale formations in Sichuan Basin, China, is volatile oil, which has greater movability compared with other types of oil. However, the production practice showed that the oil production rate declined significantly at the primary production stage (produced by depletion). Therefore, measures of enhanced oil recovery (EOR) should be implemented to acheive effective shale oil production. Carbon dioxide (CO2) huff 'n'puff has been widely used to improve the recovery efficiency of shale oil. Meanwhile, CO2 storage can be acheived by injecting CO2 in shale oil formations. In this study, a field-scale numerical model was established based on the real geological conditions and formation properties of the Sichuan Basin, China, and the model was validated by history match of shale oil production data. Molecular diffusion of CO2, confinement of nanopores, adsorption of CO2, and solubility of CO2 in water were considered in the numerical model. Effects of injection rate and time, time span of soaking, number of huff 'n'puff cycles on the shale oil production were investigated by sensitivity analysis. Results showed that the molecular diffusion of CO2 and confinement of nanopores helps to increase the efficiency of huff 'n'puff of CO2, The adsorption of CO2 on the surface of nanopores and the dissolution of CO2 in water and oil contribute to increase the amount of CO2 storage in shale oil formations. In addition, the earlier injection of CO2 leads to higher oil recovery, and five cycle CO2 huff 'n'puff can enhance the oil recovery by 11.67%, with 40% of the injected CO2 stored in shale oil formations .When the time span of CO2 soaking time exceeds 30 days, the increase oil producution is not significant. This work provides an important guidence for the effective EOR of volatile oil by CO2 huff 'n'puff in shale oil formations..

Keywords : Shale oil formations, CO2 huff ‘n’Puff, EOR of volatile oil, CO2 storage, numerical simulations.

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MS11 / 412

Microfluidic platform studying transport dynamics in weathering crust soil

Authors: Bowen Ling[1]; Enhao Liu[2]; Gaofeng Wang[2]; Hongping He[2]; Jianxi Zhu[2]; Wei Tan[2]; Xiaoliang Liang[2]

[1] *Institute of Mechanics, Chinese Academy of Sciences*

[2] *Guangzhou Institute of Geochemistry, Chinese Academy of Sciences*

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Microfluidics provides an excellent technology for studying fluid flow and solute transport in porous media with high temporal-spatial resolution, making it possible to observe fluid movement in the pore network. However, microfluidic chips are typically composed of artificial materials such as polymer, silicon, and glass, with limited research incorporating natural samples. This has hindered the progress of microfluidics. This study introduces a new microfluidic platform that encapsulates natural soil samples of weathering crust. By utilizing an inverted microscope, flow and transport dynamics in the natural soil were observed at the pore-scale with varying levels of saturation. As saturation increased, the fluid moved more easily through the pore network, and the solution diffused more rapidly. This newly developed microfluidic platform enables researchers to reveal complex transport dynamics in natural media.

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MS10 / 413

Pore fluid identification with innovative non-electrical methodology for Ultradeep tight reservoirs

Authors: Liang Cai[None]; Shengquan Ge[None]; Shichen Shuai[None]; Wei Zhang[None]

Corresponding Author: lcai@slb.com

The Tarim Basin is well known for its high-gas production as observed in the remarkable West-to-East Gas Transmission Project. The reservoirs are mainly located deep at approximately 8000-m vertically in different types of lithologies, with tight petrophysical properties. Fluid identification is a key tool used to locate the sweet spot with high producibility for further development. Resistivity is the most common and straight-forward method for identifying the sweet spot. However, because of the mixed effects from pore structure, formation sedimentary dips, far-end fractures, and the influence of the surrounding rocks etc., hydrocarbon and water cannot be easily distinguished based on the resistivity difference. In tight carbonates, the Archie equation is not always a good solution while the reservoir shows strong heterogeneity in mineralogy and pore structure. There is no obvious cross-over effect for sonic based analysis as well. This paper presents how a novel methodology based on nonelectric openhole logs reveals the fluid types in the tight sandstone and carbonate reservoirs in this ultradeep environment.

The workflow presented in this paper is based on wireline logging techniques, including advanced spectroscopy and nuclear magnetic resonance (NMR) T1-T2 measurements. Advanced spectroscopy uses both capture and inelastic gamma ray spectroscopy measurements, providing precise dry weights for elements and minerals, together with total organic carbon (TOC). The spectroscopy measurements also provide the thermal neutron cross section (sigma) and chlorine concentration measurements, which are sensitive to different fluids while the formation is saline. T1-T2-based 2D NMR measurements provide porosity and permeability information for T2-based analysis. When used in conjunction with T1 -based measurements, the fluid identification through different T1-T2 response provides an advantage for distinguishing hydrocarbons and water. Relaxation due to diffusion only applies to T2 and never to T1. Given the typical magnetic field gradients of the logging tool, the oil and gas signal can be easily distinguished from the T1/ T2 ratio. The continuous measurement enables separation and quantitation of different fluids that exist in the pore system for the entire interval of the targeted reservoir.

This paper presents case studies from this ultradeep reservoir in China for both clastics and carbonates formations that solved the fluid identification issue when resistivity cannot directly distinguish fluid types. For hydrocarbon zones, borehole and formation chlorine concentration without obvious difference, and for T1/T2 ratio is normally over three summarized from different formation types. The results matched well with the test results, which provided a novel solution to f the sweet spot interval identification for the targeted reservoir. The results show the compatibility of this workflow in different formation types and reservoirs.

This paper presents a successful and novel integrated workflow that combines multiple wireline measurements for fluid identification in tight carbonate reservoirs when the uncertainty of the resistivity method is high due to multiple factors. Also, the nonelectrical methodology significantly lowers the uncertainty for water saturation estimation. This result has helped to enhance the methodology for fluid identification and earn considerable economic value by escaping the water zones in the further development of the reservoir.

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414

Analysis and Mathematical Characterization of Subsurface CO2 Dissolution and Storage Mechanisms Using Microfluidic Technology

Author: zheng chen[1]

Co-authors: Yuliang Su ; lei li ; Xue Zhang ; Yongmao Hao

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The subsurface sequestration of CO2 in saline aquifers has garnered significant attention as a pivotal technology for mitigating climate change. This study focuses on employing microfluidic technology to investigate the dissolution and storage mechanisms of CO2 below the Earth's surface, with a specific emphasis on understanding the effects under diverse salinity, temperature, and pressure conditions. The research aims to utilize microfluidic technology and mathematical methodologies to elucidate the mechanisms governing CO2 dissolution and storage at various salinity levels.

To achieve this objective, a microfluidic experimental system was designed to replicate subsurface saline aquifer conditions, incorporating variations in salinity, temperature, and pressure. By applying Eyring theory, a comprehensive mathematical model was formulated to consider the influences of temperature, pressure, and salinity on CO2 dissolution. Furthermore, mathematical parameters were introduced to characterize diffusion and chemical reaction processes under different pore diameters. Finally, employing a porous media model, the study quantifies the range of CO2 dissolution diffusion and storage mechanisms under distinct conditions.

The experimental outcomes reveal a mere 5% average absolute error between the diffusion coefficients calculated by the mathematical model and the experimental data. The diffusion coefficient of CO2 in saline water increases with temperature elevation and decreases with rising salinity, indicating that pore space constrains the dissolution diffusion. Non-uniform pore distribution may lead to uneven CO2 diffusion, with the maximum diffusion range observed under the study conditions (50℃, 20MPa) being 15.6μm. Elevated temperature and pressure amplify CO2 diffusion, while higher salinity promotes a more uniform diffusion.

This study systematically investigates the subsurface dissolution and storage of CO2 in saline aquifers using microfluidic technology and mathematical modeling. With a focus on the impact of salinity, temperature, and pressure, experimental validation affirms the accuracy of the established mathematical model, demonstrating that higher temperature and pressure expand the CO2 diffusion range, and increased salinity results in a more uniform diffusion. The research provides crucial experimental and simulation support for a deeper understanding of the mechanisms behind subsurface CO2 dissolution and storage, with significant implications for environmental science and climate change regulation.

Keyword: CO2 sequestration in saline aquifers, CO2 dissolution storage, diffusion coefficient, microfluidic technology, mathematical characterization

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MS11 / 415

Pore-scale investigation into the effects of fluid perturbation during hydrate formation

Author: Rui Xu[None]

Co-authors: Jian-Wu Liu ; Xiao-Sen Li ; Yi Wang ; Yu Deng ; Zhao-Yang Chen

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In order to increase the gas production efficiency during methane hydrate exploitation, the research focus should be on the methane hydrate formation and decomposition mechanism nowadays. As methane hydrate reformation and the hydrate heterogeneity in the pore of sediments show great influence on gas production during hydrate decomposition, new insights need to be supplemented to reveal the mechanism of hydrate phase transition. In this work, a new microfluidic chip "simple straight pipe chip"was designed based on the microfluidic device. By comparing with the former chip "cylindrical structure chip", a series of experiments was conducted to investigate the morphology of hydrate phase transition. The "water perturbation under gas-filled situation"method and the "gas perturbation under water-filled situation"method were applied for hydrate formation. The results connect different methane hydrate growth patterns to different occurrence patterns in hydrate-bearing sediments. In the gas-filled situation, with the water migration rate rising, the hydrate stable state varies from grain-coating hydrate to load-bearing hydrate. In the water-filled situation, with the gas migration rate rising, the hydrate stable state becomes narrower. These results also gave explanations for hydrate reformation and heterogeneity in hydrate-bearing sediments. The depressurization in gas production will create water and gas flow to varying degrees, which will lead to hydrate reformation and the heterogeneity situation. Finally, these findings also provided valuable information and data for gas production and further research into gas hydrate.

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Poster / **416**

Simulation of the Microscopic Three-Phase Flow Process in CO2 Miscible Flooding at the Pore Scale

Authors: Jing Li[1]; Chuanzhi Cui[1]

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CO2 flooding after water flooding can effectively improve the recovery efficiency of low-permeability reservoirs. At present, the seepage law of CO2 flooding after water flooding is generally determined through indoor core experiments and macroscopic numerical simulation methods, and simulations of the seepage process at the microscopic pore scale are lacking. Among the existing microscopic numerical simulation methods, two-phase flow simulation is generally the main focus, and multiphase flow simulation under the conditions of three-phase coexistence of oil, gas, and water is lacking. In view of the above problems, this paper conducts a microscopic numerical simulation of the CO2 flooding seepage process after water flooding based on a two-dimensional heterogeneous pore model of circular media and studies the effects of interface tension and injection velocity on the three-phase seepage process, gas breakthrough time, and gas recovery degree during the multistage miscible process. The research shows that when the interfacial tension between CO2 and oil is high, CO2 pushes water and oil forward in a piston-like manner and penetrates the water layer to contact the oil, which ultimately causes the continuous water phase to separate from the gas phase and form the main flow line of the continuous gas phase. With decreasing interfacial tension between CO2 and oil, i.e., closer to the miscible state, the gas diffuses into the water after injection and accumulates at the water-oil interface, the crude oil is displaced toward the production end, and the flow speed of CO2 is faster than that of the water phase. The lower the interfacial tension is, the shorter the gas breakthrough time at the outlet after CO2 injection. Before the miscible state of CO2 and oil, the lower the interfacial tension is, the earlier the gas channeling time, and the lower the recovery degree. After mixing, a turning point occurs. An increase in the injection velocity will advance the gas breakthrough time and gas channeling time at the outlet, leading to an increase in the gas recovery degree. This study has reference and guiding significance for understanding the three-phase flow characteristics of oil, water, and gas during CO2 miscible flooding in mines.

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MS08 / **417**

Dynamics of contaminant flow through porous media containing biochar adsorbers

Author: Kaj Pettersson[1]

Co-authors: Albin Nordlander [1]; Angela Sasic Kalagasidis [1]; Dario Jonsson Maggiolo [1]; Oskar Modin [1]

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Biochar is used as an additive in green roof soil substrates to aid in the regulation of fertilizer storage and dispersal, preventing unwanted runoff of the chemicals. The evolution of contaminant transport and adsorption by biochar added to a packed bed is analyzed using experiments and simulations. Experiment 1 is used to determine the equilibrium capacity and adsorption rate of two types of biochar when immersed in a methylene blue solution. Experiment 2 determines the breakthrough curves of a packed bed of glass beads with randomly interspersed biochar as a methylene blue solution is circulated. Simulations are run using the properties extracted from experiment 1 and the results are compared with experiment 2. An analytical model is proposed and utilized to mimic the behavior of biochar reaching equilibrium, unable to remove additional solute. Monodisperse beds are superior in the removal of solute but removal efficiency is heavily related to the surface area of the reactive particles and the rate at which they become unable to remove additional solute. The cases using the analytical model display a tight distribution of particle surface concentration at times after the solution front passing, indicating full immersion in the solution and therefore maximum removal efficiency. In comparison, the cases with constant reactivity display a much wider distribution of surface concentrations, indicating uneven exposure. The polydisperse beds create more channeling effects which reduce reactive particle efficiency and lead to higher breakthrough concentration profiles. Comparison between experiments and simulations show good agreement with breakthrough curves.

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Poster / **418**

Microscopic visualization experimental study of salt precipitation during supercritical CO2 injection into saline aquifers

Authors: Yongchao Wang[1]; Yulong Zhao[1]; Shaomu Wen[2]; Liehui Zhang[1]; Yuqiang Zha[3]; Zihan Zhao[4]; Tao Zhang[5]; Cheng Cao[6]

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Abstract: CO2 storage in deep saline aquifers is considered an effective means of mitigating climate change induced by increased CO2 levels in the atmosphere. Additionally, CO2 has a significant impact on enhancing gas recovery (CO2-EGR). Therefore, injecting CO2 into water-bearing gas reservoirs is a win-win way for both CO2 storage and utilization. However, CO2 injection into saline aquifers leads to salt precipitation, resulting in decreased permeability. Hence, under conditions of 20MPa and 80℃, this study conducted laboratory-scale microscopic visualization experiments to investigate the growth, distribution， and migration patterns of salt precipitation, and its impact on permeability at the pore scale.
The experimental results indicate: (1) During CO2 injection, salt precipitation grows faster within the mainstream channels while exhibiting slower growth on the sides, primarily distributing along the CO2 mainstream paths. (2) As CO2 is injected, pressure differentials rise at the inlet and outlet, and decrease after CO2 breakthrough. Pressure differentials increase after salt crystallization. Finally, and increases by a factor of 12.6 due to salt precipitation, leading to a reduction in permeability. (3) Salt precipitation in the mainstream area increases the CO2 sweep area and reduces gas channeling. Salt precipitation at the boundary between swept and unswept areas limits the growth of the CO2 sweep area. (4) Salt precipitation mainly occurs in narrow pore throats and at crossed channels. Salt precipitation at narrow throats is formed, due to the limited liquid by capillary pressure is evaporated. At a crossed channel, salt precipitation primarily is formed by the evaporation of liquid film attached to the grain and aggregation of salt particles during movement. (5) Salt precipitation at narrow pore throats occurs mainly on the sides of channels with higher CO2 velocity, while at a crossed channel, it predominantly grows facing the direction of the CO2 flow, being ‘cone-shaped’ and growing. (6) In enclosed brine, a little salt precipitation is formed as CO2 is injected. Through these experiments, the mechanisms of salt precipitation during CO2 injection are elucidated, and providing a reliable basis for enhancing water-bearing gas recovery and storage.

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MS03 / **419**

Elementary Slip Solutions for Efficient Geomechanical Simulation of Fractured Rock

Authors: Giulia Conti[None]; Stephan Matthai[1]; Patrick Jenny[None]

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The prediction of the permeability enhancement that can be achieved in a geothermal system (EGS) is challenging and computationally expensive because it requires the quantification of distributed frictional sliding and tensile opening in fracture networks with a practically relevant level of complexity. Yet, modelling these processes is indispensable for determining dynamic fracture aperture that is paramount for the predictive simulation of coupled flow, transport, and geomechanical processes in EGS.
Here we model this deformation assuming that the rock matrix is homogeneous and has a linear elasticity behaviour. Single isolated fractures sheared under a compressive stress are assumed to develop an elliptic slip profile, assuming a linear relationship between maximum slip and induced stress. We employ such simplified single-fracture solutions as basis functions in a framework that attempts to predict complex stresses by superposition. To deal with the stress singularities at the fracture tips, a modification of tip stresses is applied, facilitating correct resolution of the traction forces. Since the basis functions are generated numerically, our model is readily extended to include different slip profile shapes and basis functions; for instance, to model the stresses at fracture intersections. Overall stresses are obtained by mapping the set of basis functions to the discrete fracture domain of interest. This stress field reflects the superposition of the far field- and all slip-induced stress fields. It allows to determine the maximum slip and tensile opening value along each fracture based on local force balance constraints and therefore the fracture aperture distribution.
Importantly, our approach allows to dramatically reduce the number of degrees of freedom as compared to the discrete contact mechanics-based simulation of the same fracture geometry. This opens the door to realistically complex coupled flow and transport computations for the performance prediction of EGS.

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MS03 / **420**

Impact of corner-bridge flow on capillary pressure curve

Authors: Guan-Xiong Wang[1]; Ran Hu[2]; Tian Lan[1]; Yi-Feng Chen[2]; Zhibing Yang[2]

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The capillary pressure curve is essential for predicting multiphase flow processes in geological systems. At low saturations, wetting films form and become important, but how wetting films control this curve remains inadequately understood. In this study, we combine microfluidic experiments with pore-network modeling to investigate the impact of corner-bridge flow on the capillary pressure curve in porous media. Using a CMOS camera and a confocal laser scanning microscopy, we directly observe the corner-bridge flow under quasi-static drainage displacement, revealing that corner-bridge flow serves as an additional flow path to drain trapped water. Consequently, the capillary pressure curve shifts towards lower saturations, resulting in a reduced water residual saturation. We establish a theoretical criterion for the occurrence of corner-bridge flow and develop a pore-network model to simulate quasi-static drainage, taking into account this additional flow path. Pore-network modeling results agree well with our experimental observation. On this basis, we employ our pore-network model to systematically analyze the impact of corner-bridge flow on capillary pressure curve across varying porosity, pore-scale disorder, and system size. Results indicate that the impact of corner-bridge flow becomes more pronounced as porosity decreases and shape factor increases. Our findings demonstrate that the maximum decrease of water residual saturation is 0.19 when porosity is at its minimum, and the shape factor is at its maximum. This work bridges the gap between the pore-scale mechanism and capillary pressure behavior and has significant implications for estimating the amount of extractable water and the CO2 storage capacity.

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Poster / 421

Relationship between Pore Structure and Reaction Characteristics in Supercritical Water Gasification of Chunk Coa

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Due to the essential differences in mass and heat transfer in supercritical water pyrolysis of lump coal, this study focuses on low coalification degree lignite. Employing an organic rock supercritical

water reaction apparatus in conjunction with nuclear magnetic resonance and differential scanning calorimetry, we investigated the reaction characteristics of chunk coal supercritical water gasification under continuous water injection conditions. The study explored the influence of different temperatures, pressures, and gasification reaction times on mass and heat transfer, gas yield, and composition of chunk coal. The research outcomes reveal: 1) With increasing temperature and pressure, the specific heat capacity exhibits an initial rise followed by a decline; 2) Carbon gasification efficiency improves with prolonged reaction time, while H2 yield shows an initial increase followed by a decrease; 3) Combining nuclear magnetic resonance images with DSC curves, it is observed that with the extension of temperature and reaction time, the fractures in chunk coal increase, leading to enhanced mass and heat transfer efficiency.

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Poster / 423

Study on enhanced WAG expanding swept volume technology based on carbon dioxide thickener

Authors: Pengwei Fang[1]; Qun Zhang[2]; Zhengming Yang[3]; Zemin Ji[4]; Hongwei Yu[4]; Meng DU[3]; Xinliang Cheng[3]; Yuan Gao[3]

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Abstract: The low viscosity of CO2 and the non-homogeneity of the reservoir can easily cause early gas channeling in the reservoir, which greatly reduces the sequestration and utilization of CO2, so it is important to study the technology of CO2 -WAG flood to expand the wave and volume in the onshore non-homogeneous reservoir. Therefore, we synthesized a chemical agent for CO2 responsive thickening, which is used to expand the wave and volume of CO2-WAG flood and improve oil recovery. This paper focuses on the fluid and reservoir characteristics of strongly inhomogeneous reservoir in Daqing Aonan. Under the temperature and pressure of the target block, long core driving experiment and two-dimensional non-homogeneous microscopic visualization flooding experiment were carried out, and the effect of CO2 flooding and wave reach efficiency under different flooding methods were obtained, and the laws of CO2 flooding and wave reach and the optimal injection scheme under different injection methods in non-homogeneous reservoirs were summarized. The study shows that: ① the enhanced CO2-WAG flood in non-homogeneous reservoirs can significantly inhibit gas flushing and viscous fingering compared with the ordinary CO2-WAG flood and CO2

flood, and form a piston type stable displacement leading edge, which can significantly improve the oil/gas flow rate ratio. ② Enhanced CO2-WAG flood can improve the recovery rate of more than 8% on the basis of CO2 flood and water flood, and the foam emulsion formed can significantly increase the pressure difference between injection and extraction, and can block the advantageous channels and cracks of gas flood. ③ The enhanced WAG flood can have good utilization effect on the microscopic residual oil in the small and large orifice throats and blind ends, so the enhanced CO2-WAG flood has the highest microscopic sweep efficiency and recovery degree under the other three types of drive replacement (chemical flood, CO2-WAG flood, CO2 flood).
Keywords: enhanced CO2-WAG; non-homogeneous reservoir; different injection methods;

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MS13 / **424**

A comprehensive study on shale pyrolysis dynamics by real-time in-situ imaging technology

Authors: Xia Yin[1]; Weiyi Pan[1]; Jie Zhang[1]; Zengmin Lun[1]; Stefan Iglauer[2]; Bin Pan[3]

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Shale oil and gas primarily exist in nanoscale pore-fracture networks. Despite of the large resources of the oil shale and low-medium mature shale, limited removable hydrocarbon and extremely low permeability due to limited pores restrict in the development of those unconventional resources. Therefore, different pyrolysis technologies, such as in situ conversion pyrolysis, superheated steam, nitrogen, electrofrac and etc., were emerged to accomplish the recovery. With the pyrolysis and maturing process, the kerogen was transformed into oil and gas, and more fractures and pores were generated, which increases both the permeability and hydrocarbon in the shale.
In order to study this dynamic process, a real-time in-situ imaging via environmental scanning electron microscope was applied to characterize and analyze the nano to micro scale changes of the shale quantitatively. Afterwards, Energy Dispersive Spectrometer (EDS), Rock Evaluation, and Thermal Gravity Analysis-Fourier Transform Infrared Spectroscopy (TGA-FTIR) were conducted for the physical and chemical alternation of the shale components and expulsed fluid. The real-time in situ SEM showed that 1) nano-fractures started to appear below 100 ℃; 2) inorganic nano-fracture width demonstrated a non-monotonous relationship with temperature; and 3) kerogens amount decreased

monotonously as temperature increased, especially during 400-500oC. TGA-FTIR indicated 4 pyrolysis stages with different characteristic changes, in which main expulsed products were CO2, H2O, and light hydrocarbons C1-C5. SEM images along with EDS characterized the inorganic components and their changes after pyrolysis.
These findings will promote fundamental understanding of oil shale pyrolysis dynamics at nanoscale and provide key guidance on oil shale extraction at reservoir scale.

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MS15 / **425**

Anchored Physics-Informed Neural Network for Fluid Flow Simulation in Heterogeneous Porous Media

Author: Jingqi Lin[1]

Co-authors: Xia Yan [1]; Sheng Wang [1]; Kai Zhang [1]; Jun Yao [1]

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Numerical simulation is a vital tool for analyzing and predicting fluid flow in porous media. Physics-Informed Neural Networks (PINNs) can work out systems of partial differential equations (PDEs) by leveraging the universal approximation ability of Neural Network (NN), offering a novel approach for numerical model solving. However, current PINN-based methods are rarely used to simulate heterogeneous problems, especially in the coordinate-to-pressure mapping, where the training is challenging and the output accuracy is insufficient. In this work, we propose an Anchored Physics-Informed Neural Network (A-PINN) to tackle these problems involving complex physical backgrounds. Specifically, heterogeneous permeability fields are generated by Stanford Geostatistical Modeling Software (SGeMS). Boundary conditions are incorporated into the training process as hard constraints. The loss function is constructed by Finite Volume Method (FVM), which fixes the sampling points and eliminates the need for labeled data. We innovatively design an Adjacency-Location Anchoring(ALA) structure, which enhances the network interpretability by incorporating physical significance into the NN. Additionally, the ALA possess regularization ability during the updating of network parameters. Finally, we simulate multiple heterogeneous reservoirs to verify the superiority of A-PINN in solving complex problems. The new method can achieve sufficient accuracy and significantly improve the training speed.

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Poster / 426

Effect of pore size of electrospun membrane on quality and ion separation of nanofiltration membrane

Authors: zahra khezri[1]; Masoud Riazi[2]; Seyed Hamed Mousavi[1]

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In this research, the effect of the pore size of the electrospun membrane in the preparation of a three-layer thin film nanofiber composite membrane (TFNC) was investigated. Due to its special properties, such as high porosity and the ability to produce pore sizes ranging from tens of nanometers to several micrometers, along with different mechanical properties, it finds wide applications in various fields, including medicine and health (i.e., tissue engineering, drug delivery, protective clothing, and biosensors), environment (air and water filtration membranes), energy (solar cell, battery fuel) and makes the use of electrospun membranes highly promising in separation technology. The three-layer membrane comprised a first layer of mesh-shaped polyester and a middle layer of a substrate consisting of hydrophobic polysulfone with a concentration of 20% by weight. The middle layer was produced by electrospinning with varying pore sizes. The third layer was a polyamide layer formed through interfacial polymerization between piperazine monomers (2wt.%) and trimesoyl chloride monomers (0.2wt.%). The polyamide layer and polysulfone fibers were characterized using infrared spectroscopy (FTIR), scanning electron microscope (SEM), bubble point, and MgSO4 divalent ion separation.

Based on the FTIR test, peaks of 1618 and 2990 were observed, indicating the presence of the polyamide layer and polysulfone substrate, respectively. The electrospinning was conducted under constant conditions, including a voltage of 17 kV, a needle-to-collector distance of 120 mm, and a variable polymer injection rate set at 2, 1.2, 0.8, and 0.5 ml/h. The diameter of the fibers was measured using SEM images (0.11 ± 1.25, 0.45 ± 0.9, 0.37 ± 0.58, and 0.12 ± 0.3 micrometers), and the pore sizes of each substrate were measured as 9.3, 7.1, 3.5, and 1.1 microns by bubble point. The MgSO4 salt separation test was conducted on membranes with various pore sizes and fiber diameters after the coating process. In this experiment, the separation percentage for MgSO4 divalent salt was measured as 0%, 23%, 51%, and 83%, respectively. The separation of MgSO4 ions increased with the reduction of the pore size.

Nanofiltration is a relatively recent separation process that has found widespread applications in the chemical and environmental industries due to its lower energy consumption and higher flux. In this study, we investigated the effect of the pore size of the electrospun layer. It was observed that the average diameter of the electrospun membrane fibers has a direct relationship with the pore size. As the diameter of the fibers decreases, the pore space also becomes smaller. Subsequently, the layer uniformity of polyamide is enhanced on the electrospun membrane, leading to a higher separation rate of bivalent ions.

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427

Advanced Imaging with FIB-SEM Technology: A Case Study on Nanoscale Porous Structures in Shale Reservoirs

Author: Yunfei Zhang[1]

Co-authors: Zhaojie Song [1]; Yilei Song [2]; Yufan Meng [1]; Lichao Zhang [1]

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The changing dynamics of global energy resources demand a thorough comprehension of unconventional shale reservoirs that are contributing more and more to oil and gas production. A crucial characteristic of these reservoirs is their intricate nanoscale porous structures, which conventional imaging techniques, such as Scanning Electron Microscopy (SEM) and Micro-CT, struggle to accurately characterize. This study presents the utilization of Focused Ion Beam Scanning Electron Microscopy (FIB-SEM) as an advanced method to elucidate the three-dimensional pore networks within shale with nanometer resolution.

FIB-SEM employs a gallium ion beam to precisely slice through shale samples while simultaneously imaging the exposed surfaces with an electron beam. This sophisticated technique improves the characterization of porous structures by preventing artificial pore introduction during sample preparation, thereby preserving the authentic spatial distribution of pores for further analysis.

Utilizing Avizo and PerGeos software to reconstruct three-dimensional images, we segmented the FIB-SEM images based on grayscale values corresponding to the atomic composition of the shale constituents. Subsequent analysis involved constructing a Pore Network Model (PNM), which enabled the quantification of key features within the pore structure, including measuring pore and throat dimensions, such as radius and length, as well as calculating the coordination number. This step is essential for understanding the connectivity and flow characteristics within the shale samples' porous network.

Our investigation encompassed three distinct shale samples, revealing diverse pore network characteristics: felsic shale displayed an extensive interconnected pore network with widespread percolation channels; dolomitic shale showed moderate connectivity with some isolated pores; and hybrid shale demonstrated minimal connectivity with "trigonal cone-shaped" pores interconnected by "curved sheet" throats. The findings highlight the potential of FIB-SEM to provide a detailed quantitative assessment of shale porosity and pore structure, offering critical insights into the microstructural intricacies of shale reservoirs. Consequently, FIB-SEM serves as a pivotal tool in advancing our understanding of shale microstructure, which is vital for optimizing hydrocarbon extraction from these unconventional resources.

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MS06-A / **428**

Effect of Porous media on Minimum Miscibility Pressure

Authors: Ali Safaee[1]; Masoud Riazi[2]

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Nowadays, due to the substantial oil consumption and a significant reduction in the natural oil reservoir production capacity, the demand for methods to enhance and optimize production life, especially in mature reservoirs, has grown. Enhancing oil recovery (EOR) from mature reservoirs is a well-known technique that can meet growing energy demands. Among various EOR methods, gas-based techniques stand out as the most effective. This could be attributed to some advantages, including easier injection, higher efficiency, and reduced costs in comparison to alternative methods. In gas-based injection techniques, the minimum miscibility pressure (MMP) and enrichment (MME) are among the two determining factors for operational optimization. The impact of porous media on MMP is a key question from the scientific and operational point of view because due to the confinement of a porous media, the phase behavior of both oil and gas can vary according to the porous media characteristics, such as porosity and permeability.

The primary objective of this study is to present the Vanishing Interfacial Tension (VIT) test as an easy and fast experimental approach compared to the slim tube technique for the analysis and determination of optimal conditions in gas injection processes. This research covers the introduction of both laboratory experiments and mathematical modeling of the VIT test for a live oil sample and an injected hydrocarbon gas. This method aids in assessing the sensitivity of active mechanisms within gas injection processes to the composition of the injection gas. Furthermore, the VIT model in this study has been modified based on porous media porosity and permeability, which the results show the reduction of MMP by permeability/porosity ratio decrease, for example in one case the MMP varied from 3600 to 3200 psi by decreasing the permeability/porosity ratio from 2 to 0.1. Also, the interfacial tension of oil and gas varies from 8 to 6 mN/m. Hence, the miscibility can happen more easily by permeability/porosity ratio reduction.

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MS21 / 430

Modeling Non-Newtonian Polymer Flooding in Heterogeneous Carbonate Rock: An Experimental and Simulation Investigation

Authors: Chuangchuang Qi[1]; Mohamed Haroun[1]; Mohammed Al Kobaisi[2]; Md Motiur Rahman[1]

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Polymer flooding is a widely used chemical Enhanced Oil Recovery (EOR) technique in carbonate reservoirs that can decrease water-oil mobility ratio and thereby enhance sweep efficiency. However, the accuracy of simulating polymer flooding in porous media relies on integrated characterization on polymer properties, especially rheological behavior of polymer. The objective of this study is to accurately model and predict shear-thickening and shear-thinning behavior of polymer injection of heterogeneous porous media by incorporating Special Core Analysis (SCAL), bulk rheology test, injectivity test and coreflooding experiments.

This study started with integrated fluid and reservoir rock characterization. Injectivity tests and core-flooding experiments were then conducted, including sea water flooding and polymer flooding in low-permeability (20 mD) and high-permeability (200 mD) outcrops. The pre-constructed polymer coreflooding simulation model was history matched with experimental results and uncertain parameters were calibrated by optimizing key indicators reflecting polymer non-Newtonian behavior in porous media. The calibrated model was then used to model the polymer in-situ rheology and EOR performance in a heterogeneous core sample combining high-permeability and low-permeability layers. Nuclear Magnetic Resonance (NMR) technology was used before and after polymer flooding

to confirm the pore size distribution affected by polymer injection.
Following the rock characterization study, the base simulation model M1 was incorporated with data on porosity, end-point water and oil permeabilities, and fluid viscosity. After polymer rheology and adsorption studies, the model was upgraded to M2, which displayed increased accuracy in polymer in-situ rheology and integrity affected by adsorption. Model M2 was utilized to history match base water and polymer oil displacement efficiency experiments, and the initial match degree was evaluated. Uncertain parameters, including apparent viscosity, Inaccessible pore volume, and relative permeability curve, were then adjusted by optimizing an objective function that included pressure drop, water breakthrough time, and cumulative oil production. After multiple iterations of history match, significant improvements in accuracy were observed in the calibrated model, which was then utilized to forecast polymer coreflooding performance in the heterogeneous carbonate core sample. However, the initial match was insufficient due to the complex crossflow of polymer solution between the high permeability layer and low permeability layer. Adjustments to the vertical permeability resulted in the final model M3, which achieved a high history match degree with experimental results.
In this investigation, A polymer that has both shear-thickening and shear-thinning features was modeled and calibrated step by step based on experimental results. The outcome was the creation of highly precise simulation models with the capability of providing forecasts for polymer in-situ rheological behavior, viscous fingering phenomenon, and EOR performance in heterogeneous carbonate rock. This methodology is instrumental in advancing our understanding of the mechanisms behind the non-Newtonian flow behavior of polymers in Darcy-scale porous media through integrated experimental and simulation investigations.

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MS11 / 433

Study on the percolation mechanism and oil displacement mechanism of a mixed solution of polymer and silica nanoparticles

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Polymer flooding is one of the important means to improve oil recovery during oilfield development. However, the performance of polymers is limited by temperature and salinity, which affects their oil displacement effect in reservoirs. Recently, studies have found that a mixed solution of polymers and nanoparticles can enhance the rheological properties of polymers and improve their oil displacement efficiency, especially in harsh geological environments where this promotion effect is more pronounced. However, research on polymer nanoparticle mixed solutions is still in its early stages, and there are few articles on the rheological properties, flow field distribution, and permeation mechanism of polymer nanoparticle mixed solutions. The aim of this experiment is to investigate the rheological properties of polymer nanoparticle mixed solutions and their promoting effect on reservoir recovery. By using a high-temperature and high-pressure rheometer, the rheological properties of a mixed solution of silica nanoparticles and partially hydrolyzed polyacrylamide were analyzed. Based on the viscosity temperature relationship, creep and creep recovery, and amplitude oscillation shear response, the viscoelastic properties and shear resistance of the mixed solution were evaluated, and the influence of silica nanoparticles on the polymer network structure was studied. Due to the unique rheological properties of mixed solutions, studying the flow state of mixed solutions in the flow channel is also crucial. In this study, a microchannel particle image velocimetry system was used to study the flow field of mixed solutions in contraction channels and porous media, and combined with a micro displacement device, the basic properties of the mixed solution were linked to actual seepage. The results indicate that silica nanoparticles can form hydrogen bonds with polymer molecular chains, and through physical crosslinking, form more complex macromolecular network structures, which can improve the rheological properties of polymers under high temperature and high salt conditions; The flow field experiment shows that as the rheological properties of the mixed solution increase, a symmetric vortex will form in the contraction channel of the mixed solution, and it can exist stably. The displacement effect of the mixed solution at the blind end position in porous media is better, and the stronger the rheological properties of the mixed solution, the better the displacement effect at the blind end position; Microscopic oil displacement experiments have shown that the better the rheological properties of the mixed solution, the better the oil displacement effect in porous media, and the more obvious the equilibrium displacement effect on non-mean porous media.

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MS15 / **434**

3D Pore Segmentation and Pore-Scale Simulation by Deep Learning

Author: Haotian Li[None]

Co-authors: Bicheng Yan [1]; Billal Aslam [1]; Mahmoud Mowafi [1]; Shuyu Sun [1]

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Objectives
This study aims to optimize the characterization and prediction of permeability and relative permeability in porous media through a multi-faceted approach. The primary objectives include achieving accurate 3D reconstruction of rock core images, implementing advanced deep learning models for segmentation, and addressing computational challenges associated with the Lattice Boltzmann Method (LBM) for permeability calculations. Furthermore, the goal is to enhance scalability by training models on relatively small representative elementary volumes (REVs).
Methodology
In this work, we perform the data acquisition of rock core images through CT scanning, followed by the 3D reconstruction of multiple 2D slices. We develop deep learning-based segmentation models to enhance pore segmentation, including 3D UNet, Attention-3D UNet, and 3D UNet-transformer. To resolve the computational bottleneck of LBM for large REV, we develop 3D-CNN models to take 3D segmented pore images offered by the segmentation network as input and learn to predict labels of permeability and relative permeability curves generated by LBM solver at relatively small REVs. Once trained, these 3D-CNN models can predict rock properties on a larger REV without computational limitations.
Results
The 3D reconstruction using the 2D slices yields highly accurate representations of rock core images. Subsequent segmentation employing 3D UNet, Attention-3D UNet, and 3D UNet-transformer identify the most accurate and effective porous network, providing valuable insights into the rock structure. The segmentation model achieves scalability by efficiently predicting permeability for larger REVs by addressing the computational challenges associated with LBM. The permeability and relative permeability values determined through up-scaled predictions of the trained model closely align with LBM data, affirming the reliability and utility of the integrated approach. This research contributes a comprehensive and efficient workflow for permeability prediction in porous media, combining advanced imaging, deep learning segmentation, and permeability prediction.
Additive Information
The deep learning-based workflow developed in this work can efficiently solve the scalability limitation of physics-based solvers, such as the Lattice Boltzmann Method, as it can accelerate the computation and extend to predicting permeability in larger REVs, which is about scalability. This dual advantage of efficiency and scalability represents a notable breakthrough, highlighting the efficiency and effectiveness of our methodology in overcoming the limitations occurring in digital rock.

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Poster / 436

Effect of flow rate and fluid chemistry on Precipitation Patterns

in acidified shales

Author: qiurong Jiang[1]

Co-authors: Ran Hu [2]; Hang Deng [3]; Bowen Ling [4]; Chenxing Zhou [5]; Zhibing Yang [2]; Yi-Feng Chen [2]

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Hydraulic fracturing is an important technique used to stimulate the productivity of shale reservoirs. During the fracturing process, mineral dissolution and precipitation usually occur due to the reuse of the hydraulic fracturing fluid (HFF) in the shale reservoirs. However, the consequences of interactions between the shale matrix and the flow-back HFFs on shale matrix remain unclear. A microfluidic chip fabricated with fractured shale was used to investigate the dynamic acidification process by injecting hydrochloric acid (HCl) under pH=2, and the subsequent precipitation processes by simultaneously injecting barium chloride (BaCl₂) and sodium sulfate (Na₂SO₄) solutions under different flow rates and pH conditions. The depth of the altered zone in the shale matrix caused by acidification and the distribution of barite precipitation due to fluid mixing were observed and characterized by an optical microscope and SEM-EDS.

With the injection of HCl, the thickness of the alteration zone gradually increased, and the increase rate decreases gradually due to the increase of diffusion path . Under the condition that the total injected solution volume is fixed, the higher the injection flow rate is, the slower the increase rate of alteration zone is. When BaCl₂ and Na₂SO₄ solutions were injected under different pH conditions (pH = 2,8,11) and flow rates(q=1.2, 4, 12, 24μl/min), as the pH increases and the flow rate decreases, the precipitation rate gradually increases, and the main distribution of precipitation shifts from the acid-etched shale matrix to the shale-fluid interface near the fracture channels.

Results demonstrate that the precipitation pattern is controlled by the localized concentration of reactants and geometry of the shale matrix, depending on the injected fluid chemistry and flow condition. This study provides valuable insights into the stimulation efficiency of shale reservoirs under the coupled effects of dissolution and precipitation with different operational conditions.

Keywords: shale matrix, hydraulic fracturing fluids, acidification, barite precipitation

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MS08 / **437**

Dissolution patterns and permeability evolution in dissolving fracture under mechanical deformation

Authors: Kai Li[None]; Ran Hu[1]; Zhibing Yang[1]; Yi-Feng Chen[1]

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Fractured rock is widely present in the crust of the Earth and provides main permeable pathways. Mineral dissolution due to reactive fluid flows would enlarge the fracture aperture, and lead to different dissolution patterns and increase the permeability. However, normal stresses would cause mechanical deformation of the fracture and pressure dissolution of contacting asperities, which can further lead to fracture closure and reduced permeability. Here, we systematically study fracture dissolution processes at different normal stresses to reveal the conditions under which fracture permeability increases or decreases. First, we develop a computational model incorporating mechanical deformation, chemical reaction at the free-fracture surfaces and pressure dissolution at contacting asperities, subsequently validating it through experiments. Comparison to existing experiment demonstrate the ability of the computational model to simulate fracture dissolution under normal stress σ. Then we use the computational model to simulate more than 300 fracture dissolution processes with a wide range of Peclet number Pe, second Damkohler number Da , normal stress σ and fracture length L. We elucidate the underlying mechanisms of different dissolution modes and their permeability evolution. We establish theoretical predictions for transitions of dissolution patterns: Da_{eff} (effective Damkohler number) predicts the transition from wormhole to uniform dissolution; Λ^{-1} (thickness ratio of reaction front) predicts the transition from compact to wormhole dissolution. We further develop theoretical predictions for the increase or decrease in fracture permeability under normal stress. There are two conditions under which decrease in fracture permeability occurs: (a) $1/Da_{eff}$>2 and a_{eff}>1; (b) Λ^{-1}<32 and a_{eff}>1, where a_{eff} is effective activity of solid. In all other cases, fracture permeability will increase. This work improves our understanding of fracture dissolution under mechanical deformation and pressure dissolution and is important for many subsurface engineering applications.

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Poster / **438**

Microscopic Simulation Methods for the Movement and Effects of Nanoparticles at the Oil-Water Interface

Author: Can Ke[None]

Co-authors: Bin Yuan [1]; Wei Zhang [1]; Yue Li [1]

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Nanoparticles are widely used in biomedicine, nanoelectronics, energy devices, and Enhancing Oil Recovery (EOR) due to their unique thermodynamic properties and large specific surface area. Recent research highlights the significant impact of the adsorption and diffusion behavior of nanoparticles at the oil-water interface on interfacial properties, particularly interfacial tension. This suggests that nanoparticles hold the potential to become pivotal materials for altering the permeability characteristics of oil-water flow within porous media. The lattice Boltzmann (LB) method emerges as a powerful mesoscale simulation technique for accurately modeling multiphase flows. In this method, the color gradient model, precisely characterizing parameters such as contact angles and interfacial tension, enables the accurate simulation of oil-water biphasic systems. The Langevin-Dynamics (LD) method excels in providing a detailed force-based characterization of nanoparticles in fluids, encompassing electrostatic forces, van der Waals forces, stochastic forces, and frictional forces. This methodology facilitates the microscale simulation of particle dynamics with a comprehensive understanding of the forces acting on nanoparticles in fluid environments.

A pioneering hybrid pore-scale simulation methodology was firstly introduced for the simulation of movement of nanoparticles and oil-water, employing the integration of Lattice-Boltzmann (LB) with Langevin-Dynamics (LD) for an in-depth exploration of the interactions involving nanoparticles at the oil-water interface. Leveraging the LB method, a high-resolution portrayal of the oil-water interface is established. Subsequently, through a discrete distribution of LB forcing sources, the LD method is incorporated to capture the influences of Brownian motion, thermal fluctuation-dissipation, multi-body hydrodynamics, and particle-particle interactions.

The simulation results indicate that the diffusion and adsorption behavior of nanoparticles at the oil-water interface significantly influences the interfacial tension. The results indicate that the diffusion rate of nanoparticles in a single phase (aqueous phase) is 4 to 6 times higher than the diffusion efficiency at the interface. As the particle size decreases according to a power-law, the diffusion coefficient of nanoparticles increases according to a power-law. This implies that nanoparticles with smaller particle diameters exhibit higher mobility and are more prone to move and adsorb at the oil-water interface. Based on these findings, we firstly propose a modified Langmuir adsorption equation, adjusted for particle non-equilibrium adsorption times (τe), to characterize the impact of nanoparticles on the interfacial tension at the oil-water interface. The equation can depict the real-time variation of the oil-water interfacial tension with increasing adsorption time. Compared to the conventional Langmuir adsorption equation, the computational accuracy is improved by approximately 15%. Finally, we observed the influence of SiO2 nanoparticles and NM4 (with four dodecyl chains uniformly modified on one side) nanoparticles on the oil-water interfacial tension under different particle sizes and injection concentrations. It was found that NM4 exhibited a 1.45 times greater reduction in interfacial tension compared to SiO2 nanoparticles. Meanwhile, small-sized (15 nm) and high concentration (0.08 wt%) of SiO2 nanoparticles have a more pronounced effect in reducing interfacial tension from 24.0 mn/m to 14.1 mn/m.

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Poster / 439

Determination of the type of free gas transport in shale gas formations based on Knudsen number from molecular perspectives

Authors: Xinyi Zhao[1]; Qian Sang[1]; Hai Sun[1]; Jun Yao[1]; Mingzhe Dong[1]

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The type of free gas transport in shale gas formations includes viscous flow, slip flow, and Knudsen diffusion. These three types of transport are categorized based on Knudsen number (Kn), which is defined as the ratio between the mean free path (MFP) of gas and the pore width. The MFP of gas in nanopores is usually estimated based on the ideal gas model. However, the gas in the nanopores is not evenly distributed due to the interactions between gas and walls, and thus the gas in nanopores cannot be viewed as ideal gas, meaning the real value of Kn may deviate from the value obtained by ideal gas model. In this study, we calculated the Kn of methane (CH4) in nanopores by molecular dynamics simulations. The values of MFP in nanopores were obtained based on the trajectories of CH4. We investigated the proportions of viscous collision, slip collision and Knudsen collision, which determine the type of gas transport. By analyzing the proportions of forementioned three types of collision for different values of Kn in nanopores, a real criterion for determining the type of free gas transport was established. Results show that, at 353.15 K with the pressure lower than 50 MPa, the value of Kn of CH4 is smaller than 0.1 in the pore with the width less than 5 nm. The major type of CH4 flow is the viscous flow when Kn < 0.07, and the slip flow should be considered when Kn > 0.07. The Knudsen diffusion cannot be ignored when Kn > 0.08. The results obtained in this study are crucial for correctly determining the type of gas transport in shale formations.

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Poster / 440

Buoyancy-driven dissolution instability in a horizontal Hele-Shaw cell

Authors: Kai Li[None]; Ran Hu[1]; Yi-Feng Chen[1]; Zhibing Yang[1]; Ting Wang[None]

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The dissolution of minerals within rock fractures is fundamental to many geological processes. Previous research on fracture dissolution has highlighted the significant role of buoyancy-driven convection leading to dissolution instability. Yet, the pore-scale mechanisms underlying this instability are poorly understood, primarily due to the challenges in experimentally determining flow velocity and concentration fields. Here, we integrate pore-scale simulations with theoretical analysis to delve into the dissolution instability prompted by buoyancy-driven convection in a radial horizontal geometry. Initially, we develop a pore-scale modeling approach incorporating gravitational effects, subsequently validating it through experiments. We then employ pore-scale numerical simulations to elucidate the 3D intricacies of flow-dissolution dynamics. Our findings reveal that a simple criterion can delineate the condition for the onset of buoyancy-driven dissolution instability. If the characteristic length falls below a critical threshold, dissolution remains stable. Conversely, exceeding this threshold leads to two distinct regimes: the unstable regime of the confined domain affected by the initial aperture, and the unstable regime of the semi-infinite domain independent of the initial aperture where the instability is no longer influenced by the lower boundary. We demonstrate that the pore-scale mechanism for this instability is due to the concentration boundary layer attaining a gravitationally unstable critical thickness. Through theoretical analysis of this layer and the timescales of diffusion and advection, we establish a theoretical model to predict where the dissolution instability occurs. This model aligns closely with our numerical simulations and experimental data across diverse conditions. Our work improves the understanding of buoyancy-driven dissolution instability in radial horizontal geometry. It is also of practical significance in understanding cavity formation in karst hydrology and preventing leaks in geological CO_2 storage.

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MS11 / 441

Experimental Study of Dissolution Regimes in a Multiphase Flow Environment with Real-Rock Microfluidics

Author: Chen-Xing Zhou[1]

Co-authors: Bowen Ling [2]; Hang Deng [3]; Ran Hu [4]; Yi-Feng Chen [4]; Zhibing Yang [4]

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Multiphase flow coupled with rock dissolution is prevalent in subsurface energy applications and natural phenomena, such as karst formation, acid stimulation, and CO₂ sequestration. The interplay between multiphase flow and rock dissolution will profoundly influence the geochemical and geophysical properties of reservoir formation. Despite its importance, we still lack a thorough understanding of the coupling of multiphase flow and rock dissolution. Here, microfluidics fabricated with the geo-materials are used to study the pore-scale mechanism of rock dissolution in a multiphase flow environment. Experimental findings reveal dissolution regimes contingent upon injection rates and the channel geometries. At lower injection rates and in more homogeneous geometries, the dissolution exhibits a uniform regime. In this regime, the evolution of the rock surface aligns with classical assumptions, facilitating the prediction of long-term dissolution rates. While under stronger flow and heterogeneous conditions, the dissolution exhibits a localized regime, and the dissolution rate deviates significantly from the classical assumptions. Experimental observations identify a pore-scale barrier mechanism that suppresses the overall dissolution rate and leads to this deviation. We also proposed a theoretical model for the regime transition, which offers guidance on the prediction of dissolution rate across various dissolution scenarios.

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MS11 / **442**

Novel Microfluidic Experiments Of Investigating Permeability Impairment due to Clogging in Rough Fractures

Authors: Xusheng Chen[1]; Ran Hu[2]; Yi-Feng Chen[2]; Zhibing Yang[2]

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Fractures commonly compromise rock integrity, emerging as a primary factor in leakage within CO₂ geological storage. Injecting CO₂ into deep saline formations often induces salt precipitation (Evaporation-induced) and mineral precipitation (Chemically-induced), leading to the obstruction of fractures and impairment of reservoir permeability. To assess these effects, we devised a novel microfluidic fracture model using PMMA and rough glass. Two distinct precipitation experiments were conducted: 1) Dry CO₂ is injected at different flow rates into a brine-filled microfluidic model to address the progression of salt precipitation induced by evaporation. 2)Na₂CO₃ and CaCl₂ are concurrently injected at different flow rates into the microfluidic fracture model to prompt mineral precipitation. Utilizing confocal laser scanning microscopy, we identified two salt precipitation modes: large bulk salt crystals and polycrystalline structures. Large bulk salt crystals lead to complete clogging, markedly

diminishing fracture permeability. Flow velocity significantly influences the precipitation pattern of mineral precipitation. At high velocity, a more constricted barrier is observed, restricting mixing and reactive transport. Conversely, at low velocity, a broader precipitation zone formed, significantly reducing fracture permeability. This study enhances our comprehension of the blocking behavior of two distinct precipitation in fractures during the CO₂ geological storage.

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MS18 / **444**

4D Study of Groundwater Remediation Techniques at Pore-scale

Authors: Meezanul Islam[1]; Nathaly Lopes Archilha[2]; Pavel Kazakovtsev[1]; Tannaz Pak[1]

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Groundwater remediation is a pressing issue in the modern world. In Brazil, almost 37% of the cities are supplied exclusively with groundwater. In Pakistan, 73% of agricultural irrigation is done with groundwater (Qureshi, 2020). According to Lunardi et al., (2021) groundwater is susceptible to contamination in regions, where pollutant source, such as industry, is present.
In this work, a dataset on nZVI nanoparticle reaction with TCE (trichloroethane) is studied. TCE is a DNAPL –Dense non-aqueous phase liquid. These compounds are challenging to be removed from groundwater aquifers via conventional means, as they are almost immiscible in water, and are difficult to remove from the porous medium. Therefore, nanoparticles used for remediation of such reservoirs must be mobile, to able to reach the contaminant and react with the source of contamination. The dataset was obtained via X-ray microtomographic scanning (X-ray micro-CT) on Diamond Light Source, and allows for 4D (3D + time) study of the processes, happening on the pore-scale. For this experiment, Sibelco sand was used, along with Nanofer 25S and 25DS nanoparticle suspensions. The studies performed on methods like ones studied in this work usually do not study what is happening on pore-scale. Such study is performed by Pandey, Sharma and Saha (2022) on nZVI nanoparticle production techniques, or by Chen et al., (2021) on slow-release potassium permanganate. This highlights a knowledge gap in the modern understanding of these remediation techniques.
Segmentation process proved to be difficult due to the contrast of resulting images. This was caused by the 4D nature of the study. While this allows us to observe the processes with great precision, it was necessary to make the measurements fast. This, in turn, reduced the contrast of the resulting images. The segmentation was performed using deep learning algorithms in Dragonfly and Annotat3D, and then visualised and analysed in Avizo. Phases, identified during segmentation, included sand grains, water, TCE, nZVI clusters and gas. This is in line with the previous work on the subject

by Pak et al., (2020), performed on glass beads.
In addition to this, a new setup has been developed for column experiments. This setup gave us the possibility to investigate liquid and particle dynamics on a larger scale, across a column of approximately 36 cm long 3.5 cm in diameter. With this setup we were able to measure particle distribution through the column after several nZVI injections on different porosities. The novelty of this setup is a magnetic susceptibility sensor, which allows to assess distribution of nanoparticles along the column, as well as to measure the amount of nanoparticles produced from the tube. This method is non-invasive, which allows to re-measure the samples in case of an error, or to obtain greater precision. The objective of these experiments is to perform a series of column experiments on Sibelco sand, using the same nanoparticle suspension as in the 4D micro-CT experiment.

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MS01 / **445**

Critical Thresholds for CO2 Foam Generation in Homogeneous Porous Media

Author: Jinyu Tang[1]

Co-authors: Bing Wei [2]; Mengke Yang [2]; William R. Rossen [3]

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Long-distance propagation of foam is one key to deep gas mobility control for CO2 sequestration (Rossen et al., 2022). It depends on two processes: convection of bubbles and foam generation at the displacement front. Prior studies with N2 foam show the existence of a critical threshold for foam generation in terms of a minimum pressure gradient (∇pmin) or minimum velocity (vt,min), beyond

which strong-foam generation is triggered. Yu et al. (2020) show that the same mechanism controls foam propagation. There are few data for ∇pmin or vt,min for CO2 foam.

We conduct extensive experiments to quantify ∇pmin and vt,min for CO2 foam generation, and quantify the correlations of ∇pmin and vt,min with factors including injected foam quality (gas fraction)–fg, surfactant concentration–Cs, and permeability–K. In each experiment, steady-state pressure gradient is measured at fixed injection rate and quality, with velocity increasing in a series of steps. The abrupt jump in ∇p against vt marks the trigger of strong foam generation (see graphical abstract: N2 data on top, schematic in middle, data for ∇pmin on bottom).

In most cases, the experimental results for ∇p as a function of vt identify three regimes: coarse foam at low ∇p, an abrupt jump in ∇p (point B in graphical abstract) and strong foam at high ∇p. The abrupt jump in ∇p upon foam generation demonstrates the existence of ∇pmin and vt,min for CO2 foam. We further show how ∇pmin and vt,min scale with fg, Cs and K. The effect of K is dominant over the effects of fg and Cs. Specifically, both ∇pmin and vt,min increase with foam quality: e.g. for fg over a range 0.5 –0.9, ∇pmin rises by a factor ~ 2 –4 and vt,min by a factor ~ 4. Increasing Cs leads to decrease in both ∇pmin and vt,min by factors of less than three. ∇pmin changes considerably with permeability. Our results in consolidated sandpacks show that ∇pmin for CO2 foam scales with K as K-2, in comparison to N2 foam, where ∇pmin scales as K-1 in unconsolidated homogeneous sand or bead packs. However, the data of Gauglitz et al. (2002) for CO2 foam in Boise sandstone do not show a dependence of ∇pmin on K. The difference may be a result of the impact of heterogeneity of the Boise sandstone, since foam generation is easier in heterogeneous media.

∇pmin is about 0.17 bar/m (~ 0.75 psi/ft) for K ~ 270 mD, 2 to 3 orders of magnitude less than for N2 foam. This pressure gradient is easily attainable deep in formations. This suggests that generation is much less of a restriction for long-distance CO2 foam propagation than with N2. Foam propagation could still be challenging in low-permeability reservoirs (∇pmin ~ 10 bar/m for K = 27 mD). Nevertheless, realistic formations are heterogeneous and field application deploys alternating-slug injection. Both factors help foam generation and thus reduce the value of ∇pmin. More research is needed to determine conditions for CO2 foam propagation under those conditions.

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MS05 / 446

Pore-scale hydrodynamics influence the spatial evolution of preferential flow paths in porous media bioclogging system

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Biofilm is a universal form of microbial existence, which is formed by microbial cells and their extracellular polymers bonded to each other. It's ubiquitous in rivers, human organs and drinking water distribution systems, where microorganisms attach to the surface of particles and cause bioclogging, which often results in negative impacts. In this paper, we developed a visualization experimental system, to realize the real-time dynamic and multi-scale observation of microbial growth under different pore structure, flow rate and nutrient concentration conditions. Visualization experimental results show that microbial growth was spatially obviously non-homogeneous due to the randomness of microbial attachment sites and preferential seepage of nutrients. In the early stage of the experiment, microorganisms mainly existed in the form of suspended cells, clusters and streams, and with the growth of microorganisms, clusters gradually coalesced to form individual biofilm clusters connecting the inlet to the outlet. In the late stage of the experiment, the biofilm formed a relatively fixed structure, and the nutrient solution mainly flowed along the preferential flow paths. Under constant flow conditions, the microbial growth led to the narrowing of the preferential flow paths, and the shear stress of the fluid would cause the preferential flow paths to become wider, the competition between microbial growth and fluid shear leads to the intermittent opening and closing of the preferential flow paths.

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Poster / **447**

A novel evolutionary optimization approach via surrogate model and autoencoder for reservoir development scheme design

Author: Qinyang Dai[1]

Co-authors: Liming Zhang [1]; Kai Zhang [2]; Guodong Chen [3]; Guoyu Qin [1]; Dawei Wu [1]; Jun Yao [1]

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The underground reservoir is a typical porous system, and the oil is stored as fluid in the pores of the reservoir. The efficient extraction of oil, which is primarily dependent on the reservoir development scheme, is a significant challenge. However, traditional reservoir development optimization methods mainly rely on manual experience or limited numerical simulation-based comparisons of development schemes. Typically, the issue of a reservoir development scheme optimization is high-dimensional when the reservoir is complicated. The proposed surrogate-assisted and autoencoder-based evolutionary optimization framework is ideally suited for addressing this challenging problem in reservoir development scheme optimization. This work intends to improve the cooperative optimization capability balancing exploration and exploitation. The autoencoder is used to map the decision space to the low-dimensional space for evolutionary optimization, thereby maximizing the value of the solutions with relatively poor performance. Surrogate model is utilized in the original high-dimensional space to pre-screening for quickly recommending new promising solutions, which further boosts the searching performance. Through the cooperation of autoencoder and surrogate model, the optimization performance for the reservoir development scheme is strengthened. This approach is tested in the reservoir cases, and the experimental results show the obtained development scheme can get more oil from the reservoir porous system. Therefore, the approach has a lot of potential for dealing with reservoir development scheme optimization design issues.

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MS06-B / 448

Enhanced CO2 Storage in Saline Aquifer by Electric Field Considering Formation Wettability

Authors: Liangyu Zhao[1]; Zheng Li[1]

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Geological CO2 storage involves injecting captured CO2 into various geological formations, in which saline aquifers have the largest storage potential around the world. In the context of carbon neutrality, one of the key issues is to store CO2 as much as possible on the premise of formation stability. In this paper, we find that external electric field can enhance CO2 storage in saline aquifers. The different mechanisms of CO2 storage enhancement in hydrophobic and hydrophilic formations are

revealed by molecular dynamics simulations. The following conclusions can be drawn. (1) In order to consider formation wettabilities, a carbon-based pore wall, a hydroxylated quartz pore wall and a calcite wall are constructed. CO2 tends to accumulate more readily on carbon-based wall, while H2O exhibits a higher tendency to accumulate near hydroxylated quartz wall and carbonate wall, indicating different wettabilities of the three walls. (2) On a short time-scale, CO2 is stored in adsorbed and dissolved states in saline aquifers of hydrophobic and hydrophilic formations. (3) In the absence of an electric field, the dissolved CO2 accounts for 42.50% in the hydrophobic formations; the adsorbed CO2 accounts for 12.4% in the hydrophilic quartz formations. When an external electric field is applied vertically to the wall, the proportion of dissolved CO2 in the hydrophobic formations increases to 63.23%; the proportion of adsorbed CO2 in the hydrophilic quartz formations increases to 21.76%. However, the external electric field has negligible effects in the hydrophilic carbonate formations. (4) The orientation of H2O molecules and the hydrogen bonds are further analyzed to reveal the different enhancement mechanism. In the hydrophobic formations, the external electric field induces oriented H2O molecules, leading to their preferential accumulation near the wall, rendering the initially hydrophobic wall hydrophilic, thereby reducing the available space for adsorbed CO2 and promoting its dissolution in the H2O phase. In the hydrophilic quartz formations, the external electric field drives H2O away from the surface, concurrently reducing the number of hydrogen bonds formed between H2O and the hydrophilic wall by approximately 24.22%. This reduction diminishes the hydrophilicity of the wall. In the hydrophilic carbonate formations, there are no hydrogen bonds between H2O molecules and the wall. Therefore, the electric field has negligible effects on the wettability of the wall and CO2 storage. This study proposes a novel technique to enhance CO2 storage in saline aquifers of different wettabilities by electric field. The molecular perspective revealing the enhancement mechanism is expected to provide theoretical guidance in the future practical application.
Keywords: Geological CO2 storage; electric field; molecular dynamics simulation;

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Poster / **449**

Modeling of CO2-Foam Rheology for Improved Injectivity Prediction in CCUS Processes

Author: Jinyu Tang[1]

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Foam is appealing for carbon sequestration due to its remarkable effectiveness in gas-mobility reduction and thus gas sweep improvement (Rossen et al., 2020). Nevertheless, the considerable gas-

mobility reduction by foam in the near-well region imposes a concern over foam injectivity. Shear-thinning rheology helps injectivity. Kim et al. (2005) and others show that CO2 foam is strongly shear thinning, with respect to both gas (Ug) and water (Uw) superficial velocities at low foam quality (fg, volumetric gas fraction in foam), as seen from the lower left figure of the graphical abstract. The shear-thinning behavior with respect to Ug has been represented in the widely used foam model, STARS (Computer Modeling Group, 2015). However, no currently applied foam models have yet accounted for the shear-thinning rheology of foam with respect to Uw. Such behavior features upward-tilting pressure-gradient contours with increasing Uw (see the graphical abstract, lower-left figure). Effective modeling of foam rheology is in particular crucial to accurate prediction of foam injectivity. Otherwise, the injectivity would be underestimated, misleading feasibility evaluation of a foam injection process.

Kim et al. (2005) identify a cause for the non-Newtonian foam rheology at wet conditions based on drag force on foam films (Hirasaki and Lawson, 1985): wet conditions create thicker water films along pore walls, leading to a reduction in drag force. In this study, we investigate how to incorporate this effect into the widely used STARS model. Specifically, a simple, semi-empirical equation is developed as a function of water saturation, to relate the effect of drag force to water saturation. The parameters involved in the equation can be easily estimated by fitting to steady-state foam data. The procedure for fitting model parameters is given and illustrated with examples (see fit to data in graphical abstract, left figure, in right figure). We also show how to couple this equation with the STARS foam model. The modified STARS model, incorporating the drag-force mechanism, is tested by fitting to steady-state data for both N2 and CO2 foam. The improved fit to the data verifies the validity of the new algorithm in representing foam rheology at low qualities (wet conditions).

In field applications, foam is usually injected through a surfactant-alternating-gas (SAG) slug mode. The injectivity of the process is primarily dominated by the injectivity of liquid slugs. Gong et al. (2020) using X-ray CT imaging of corefloods reveal that liquid injection forms fingers through in-situ foam and dissolves CO2 nearby, improving its injectivity. In addition to that, the shear-thinning rheology of foam further improves the injectivity. Therefore, considering these mechanisms improves the prediction accuracy of the injectivity of SAG foam processes. Further research is needed regarding the effect of foam rheology on liquid injectivity on the field scale.

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MS15 / 450

A Vision Transformer for Size-Agnostic Modelling of Two-Phase Drainage in Complex Porous Media Considering Wettability, Interfacial Tension, and Resolution

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The estimation of pore-scale multiphase flow fields in complex geometries using deep learning has proven challenging. This is partly because researchers have historically focused on model architecture and data quality, while the volume and variety of data may have been inadequate to capture the intricacies of multiphase flow. In this work, we introduce a novel deep learning methodology to predict phase distributions within realistic porous rocks during two-phase capillary-dominated drainage. We use Computerised Tomography (CT) images and incorporate pressure gradient, resolution, wettability (contact angle), and interfacial tension as inputs without relying on complicated expert-crafted features.

To create ground-truth datasets, we extract subsamples from CT scans of both synthetic and real rocks, including sandstones and carbonates. Primary drainage is then simulated in these sub-images by an in-house Pore Morphology-based Simulator (PMS), yielding millions of fluid occupancy instances. To maintain both pixel-wise accuracy and physical fluid connectivity, we devise a Higher-Dimensional Vision Transformer (HD-ViT). We train the model on phase distributions where the wetting phase is drained from pores solely based on their sizes, regardless of their relation to other pores and the inlet, allowing the network to focus on subtle details such as generating valid fluid-fluid interfaces. Fluid continuity is then enforced as a post-processing step by removing patches of the invading phase that are not connected to any desired inlet(s). This approach facilitates efficient inference for images of varying sizes and resolutions with any inlet-outlet setup. After training on a massive dataset of images and rock-fluid data, the model achieves outstanding results with a testing F1 score and saturation correlation coefficient above 0.95.

We confirm the model's validity by demonstrating consistently high performance on larger images of unseen sandstone and carbonate rocks through an effective patch-and-stitch strategy. The model maintains accuracy across a wide range of scales, from microns to centimetres, within the range of properties used in this study. Such scalability enables distributed computing, facilitating the processing of extremely large images. Therefore, the reported methodology can be considered a solution to the computational constraints encountered for large images. Interestingly, the HD-ViT proves even faster than the PMS, itself considered one of the most efficient simulators of drainage. This underlines the immense potential of models trained at scale, like ours, to be fine-tuned for computationally intensive simulations using smaller datasets, where the speed advantage becomes increasingly significant.

Our final model introduces multiple innovative aspects. Firstly, setting it apart from similar models, ours incorporates all factors influencing capillary drainage as inputs, offering a comprehensive approach. Secondly, the model is trained on a dataset of unprecedented size and diversity, comprising millions of highly heterogeneous and realistic images. Thirdly, by avoiding complex feature engineering, we ensure an end-to-end, easy-to-use model. Fourthly, we implement a simple and effective strategy to enforce phase connectivity in fluid distributions and to also allow for size-agnostic predictions on any inlet-outlet configuration. As such, the HD-ViT is a multiscale, practical, and efficient model for pore-scale drainage.

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Poster / 451

Understand Advection-Dispersion and their Relationship with the Scales of Heterogeneity through Lattice Boltzmann simulations

Authors: Han Tang[1]; Tian-Chyi Jim Yeh[2]; Yanhui Dong[None]

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The classical advection-dispersion equation has been a cornerstone in aquifer solute migration studies for decades. However, prevailing misunderstandings regarding advection-dispersion dynamics, their interplay with heterogeneity scales, the nature of ensemble averages, and their observational implications have sparked intense debate concerning the equation's conceptual validity. Addressing these controversies is critical for demystifying phenomena such as macrodispersion, anomalous dispersion, and scale-dependent transport, as well as for evaluating contemporary models like the dual-domain dispersion model for solute movement in aquifers. This investigation employs the Lattice Boltzmann Method (LBM) for simulating solute transport within heterogeneous porous media. Our study delineates the evolution of the dispersion concept from molecular diffusion to encompass fluid dynamic effects caused by variations in scale-specific velocities and discusses the limitations of extending Fick's law for molecular-scale velocity variations to describe the effects of large-scale velocity variations.

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MS01 / **452**

Parallel numerical simulation analysis of the stress evolution within the full synthetic field model during CO2 geological storage

Author: Enyi Yu[1]

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The mechanical analysis and stability assessment of reservoir-caprock systems are critical considerations for the successful industrial implementation of CO2 geological storage. Injecting CO2 into the formation can cause fluid pressure accumulation, altering the effective stress field and subsequently leading to potential geological risks. Stress changes due to CO2 injection can activate faults, induce seismicity, and ground motion. However, the influence of stress change is not limited to the reservoir alone but extends to the broader subsurface formations including the overlying caprock, underlying basement, and the surrounding strata.
In this study, a full synthetic field model incorporating the reservoir, caprock, basement, and surrounding formation was established. A finite element grid was generated based on the existing corner point grid of the target reservoir. Using parallel computing, numerical simulations of coupled flow and geomechanics were conducted on a million-grid scale model to analyze the variations in effective stress during CO2 injection and storage. The simulation results indicate that during the injection stage, fluid pressure and shear stress gradually increase with time, while the average effective stress decreases, indicating a shift towards the failure envelope. After the cessation of injection, the stress state reverses but remains on the left side of the initial stress state. Fluid pressure and shear stress are higher than the pre-injection equilibrium values, while the average effective stress is lower. Increasing the number of CPU cores significantly reduces the computation time of the numerical simulations. However, beyond a certain number of cores, the overall parallel computation time increases due to increased communication burden among processors. As the size of the solving model increases, the acceleration ratio and parallel efficiency increase under the same number of processors.

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Poster / **454**

Impact of wettability on supercritical CO2 transport and local capillary trapping in deep saline aquifers

Author: Xiyi Peng[1]

Co-authors: Yanyong Wang [1]; Yongming He [1]

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Given its immense storage capacity, geological CO2 storage in saline aquifers is regarded as a promising and practical strategy for mitigating anthropogenic CO2 emissions into the atmosphere. During the post-injection phase, where CO2 migration is primarily influenced by buoyant force, local capillary trapping emerges as a crucial mechanism for effective storage. In practical scenarios, saline aquifers may exhibit varying degree of wettability, leading to variation in two-phase flow of CO2 and brine, as well as capillary pressure. However, the previse understanding of how wettability influences the local capillary trapping of CO2 during buoyancy dominated flow in saline aquifer remains unclear. In this study, we firstly construct typical heterogeneous aquifer models using geostatistical modeling. Subsequently, we develop relative permeability curves and capillary pressure curves for CO2-brine in rocks with different wettability characteristics, such as water-wet, intermediate-wet, and CO2-wet. The transport and local capillary trapping of supercritical CO2 in aquifers featuring various wettability are then investigated through high-resolution two-phase flow simulations. The spatial and temporal evolution of CO2 plume is analyzed and the contribution of different trapping mechanisms, namely local capillary trapping, residual trapping, and dissolution trapping, are compared. The advantageous wettability characteristics conducive to local capillary trapping of CO2 in saline aquifers are unveiled. The findings of this study offer valuable insights into the transport and trapping mechanism of supercritical CO2 in deep saline aquifers with different wettability characteristics.

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MS15 / **455**

Optimizing Underground Hydrogen Storage through Surrogate Modeling: A CNN-LSTM-Attention Network Approach

Authors: Zhilei Han[1]; Bicheng Yan[1]; Zeeshan Tariq[1]; Zhao Feng[2]; Shuyu Sun[1]

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Underground hydrogen storage (UHS) presents a viable solution for storing excess energy in suitable geological sites, ensuring a stable and scalable energy supply 1. While extensive experience exists in underground natural gas storage 2, the significant differences in the properties of hydrogen pose unique challenges [3]. To deepen insights into the hydrogen recovery in UHS projects, conducting reservoir simulation and optimization to pinpoint optimal operating parameters becomes essential. However, this process is typically time-consuming. The integration of a surrogate model proves invaluable in expediting the optimization process, addressing the significant time constraints associated with traditional methods.

We develop a base UHS simulation model with a 3D heterogeneous depleted natural gas reservoir featuring an anticline structure. The model integrates various physics, encompassing compositional fluid flow, hydrogen methanation reaction, gravity segregation, hysteresis, and capillary effects. The cycling schedule starts with an initial phase of cushion gas injection and idle periods, followed by five distinct hydrogen injection-idle-production cycles spanning five consecutive years. Notably, injection rates and bottomhole pressure (BHP) of the production well vary across these cycles. The base model incorporates diverse cushion gas types and layers of perforation. Upon parameterizing these decision variables and employing the Latin-Hypercube method for sampling, we generate a comprehensive database comprising approximately 1000 simulation cases, executed in parallel. To predict cumulative productions of hydrogen and other components, we train a surrogate model utilizing a CNN-LSTM-Attention network, leveraging the NVIDIA RTX A6000. The CNN component transforms 3D heterogeneous permeability and porosity fields into 1D datasets. This well-tailored surrogate model seamlessly integrates into the optimization workflow based on the stochastic simplex approximate gradient (StoSAG) [4] method. The primary optimization objective is to maximize hydrogen recovery while concurrently minimizing losses attributed to micro-bio reactions within a predefined timeframe.

Due to gravitational segregation in the base model, hydrogen, cushion gas, methane, and water exhibit a vertical distribution from top to bottom. Additionally, we note a progressive enhancement in hydrogen recovery efficiency with consistent injection rates during production. Our numerical experiments highlight nitrogen's superior effectiveness as a cushion gas for augmenting hydrogen recovery compared to carbon dioxide and identify a specific percentage of micro-bio-induced hydrogen loss. Regarding the performance of the surrogate model, the R2 scores for both training and testing datasets mostly exceed 0.95, affirming its robustness and feasibility. To demonstrate the acceleration achieved through the proxy model in optimization, we compare CPU times between the reservoir simulation and surrogate models. The former averages 210-300 seconds per case, while the latter ranges from 0.01 to 0.1 seconds. This translates to a remarkable speedup of approximately 1000 times compared to optimization conducted solely with reservoir simulation, all while maintaining equivalent accuracy.

This research introduces a comprehensive framework designed for reservoir simulation and optimization in UHS, integrating a CNN-LSTM-Attention network and StoSAG. Important mechanisms, including compositional flow, cushion gas dynamics, and micro-bio reactions, are thoroughly incorporated in the UHS simulation. This framework serves as an important guideline, offering crucial insights into accelerating the optimization of the UHS process and related projects.

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MS11 / **456**

Study on Oil Displacement Mechanism of Polymer Microspheres Based on Microfluidic Technology

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Co-authors: Junjian Li [1]; Hanqiao Jiang [1]; Shuai Yuan [1]; Fuwei Yu [2]; Hang Su [3]

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As a novel type of profile control material, polymer microspheres have the characteristics of easy for injection, able to blockage and movable, which make the application in oil production has gradually expanded. This article is based on microfluidic experiment, combined with fluorescence component tracer technology, to clarify the oil displacement mechanism of polymer microspheres from a microscopic perspective.

Polymer microspheres with fluorescence properties are selected as experimental materials, and ideal microscopic models with simple channel pattern are used to conduct experiments under fluorescent and non-fluorescent conditions respectively. The mechanism of polymer microspheres is studied from three aspects: aggregation rules, migration characteristics, and morphological changes. The typical reservoir channel models are designed and made based on casting thin sections. And the effect of polymer microspheres flooding is evaluated through displacement experiments. Then using the previous conclusions to explain experimental phenomena, and the accuracy of the oil displacement mechanism is further demonstrated.

It is found that the polymer microspheres tend to act as emulsion aggregates during the displacement process. Part of microspheres injected tend to accumulate at the inlet end, and the other microspheres successfully injected into the model will enter the relatively high-permeability region along the dominant water channeling channel. After the hydration and expansion of microspheres, the particles are interconnected, forming a “microsphere partition” to block the subsequent water flow, and changing the direction of fluid flow, thereby expanding the sweep area to enhance oil recovery. With the increase of injection time, the effect is affected by the degradation failure or the desorption movement of the microspheres. Polymer microspheres exhibit varying degrees of stimulation effects in different types of reservoirs, but they are more suitable for blocking channels with high permeability in relatively homogeneous reservoirs. Therefore, the matching between the blocking agent and the channel should be fully considered when selecting the blocking adjustment measures to further improve the effectiveness of the scheme design and parameter setting.

In this paper, the oil displacement mechanism of polymer microspheres is clarified and its accuracy is verified. This understanding is of great significance for the interpretation of experimental phenomena, the improvement of numerical simulation methods and the explanation of field application effects. It also provides reference value for the optimization of microspheres application scheme design and the adjustment of on-site implementation measures.

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Poster / 457

Numerical modelling of polymer support fluids permeating in sands

Author: Si Suo[1]

Co-authors: Martin Blunt [1]; Catherine O'Sullivan

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Polymer fluids, a blend of polymers in water, offer a cost-effective and environmentally friendly solution for supporting deep underground excavations. However, being non-Newtonian fluids, their full potential in construction projects is hindered by a limited understanding of their behaviors. In this study, we will employ a combined approach of DEM-based and micro-CT imaging techniques to explore the pore-space topology in sands. Utilizing this data and considering the fluid-solid interaction, we will then develop a fully-resolved numerical model to comprehensively investigate the distribution pattern of strain and stress within the fluid phase, as well as drag forces on sand particles. Our numerical results will be validated against large-scale experimental observations, and provide insights for the development of upscaling modelling techniques.

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MS01 / **458**

Solar energy storage in saline aquifers: Insights from coupled hydro-thermo-mechanical modeling

Author: Yanyong Wang[1]

Co-authors: Kunpeng Zhong [1]; Xiyi Peng [1]

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The utilization of saline aquifer for solar energy storage is recognized as a promising solution to address the spatial and temporal mismatch between energy demand and supply. This approach holds significant potential for future renewable energy storage and conversion. Thermal energy storage in saline aquifer can effectively transform intermittent solar energy into stable geothermal energy at high temperatures. In this study, we examine a previously proposed solar energy storage and conversion system. This system entails the initial conversion of solar energy into heat through parabolic troughs, followed by the storage of thermal energy in a saline aquifer facilitated by high-temperature hot water circulation. Currently, the impact of poroelasticity and thermal stress induced by high-temperature hot water injection on injectivity and heat storage efficiency remains unclear. In this study, three-dimensional porosity and permeability fields for typical saline aquifers are generated by geostatistical modelling. The circulation of high-temperature hot water in the aquifer by doublet vertical well system is explored through coupled hydro-thermo-mechanical modeling. We analyze the effects of poroelasticity and thermal stress on the injectivity of hot water. The influences of in-situ stress and permeability heterogeneity on spatial and temporal evolution of hot water zone are then explored. In addition, the efficiency of solar energy storage in various heterogeneous saline aquifer is evaluated and compared. Considering the hydro-thermo-mechanical coupling effects, saline aquifers conducive to solar energy storage are identified. This study enhances our understanding of the mechanisms involved in solar energy storage in saline aquifers, providing crucial insights for its practical implementation.

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Accounting for non-Darcy fluid flow in porous media from a pore-scale entropic particle transport perspective.

Author: Alexandros Stamatiou[1]

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The description of fluid flow in tight porous media presents a formidable challenge with wide-ranging applications in science and technology. A fundamental problem is the correct prediction of the mass flux when the fluid is subjected to an external driving force. Experimental studies of pressure-driven fluid flow on porous samples reveal the existence of a non-linear relationship between the observed fluid velocity and the imposed pressure gradient in the low gradient region. As shown in a recent work, this sample-scale non-Darcy flow regime could arise collectively from nonlinear flows in individual pores due to the motion of fluid particles being influenced by the longitudinal geometric variations of each pore. This is equivalent to the particles undergoing biased Brownian motion, subject to a pore geometry-dependent entropic potential and an applied driving force. In this presentation, we highlight key theories in which the geometric effect is considered in modelling the biased particle diffusion and several results that relate pore-scale and sample-scale nonlinear flow. Moreover, we focus on the evaluation of the Stratonovich formula for determining the average particle velocity for a cylindrical pore with non-smooth periodic pore-wall profiles. We believe that such cases have been reported erroneously in the literature and show that the errors can be significant in comparison with those obtained by our correct evaluations. The entropic particle diffusion perspective and related techniques shown here opens an avenue for accounting for the impact of the pore geometry on the manifestation of nonlinear flow from pore to sample-scales within the pore scale modelling of realistic porous media.

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MS07 / 461

A Lagrangian Simulation Framework for Multiphase Flow and Transport in Fractured Porous Media

Author: Ranit Monga[1]

Co-authors: Daniel Meyer [2]; Patrick Jenny

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Particle tracking schemes, including random walk (RW)-based methods, are attractive for modeling advective transport, since they do not suffer from numerical diffusion [Salamon et al. (2006)][1]. In scenarios involving multi-species transport, these schemes meticulously capture the degree of spatial mixing across all scales. With such schemes, one can leverage thermodynamic rate laws which when

applied to particles in close proximity result in realistic reaction rates. This stands in contrast to classical upscaling-based approaches which assume complete mixing and may not accurately model small-scale variations in reaction rates [Ding et al. (2013)][2].

We present an improved stochastic particle method in the context of multiphase transport in fractured porous media. Our study focuses on limit case scenarios where the microscopic processes, such as capillary diffusion and pore-scale dispersion, do not exert significant influence at the macroscopic levels. For a time-varying system that exhibits a potential solution discontinuity, such as the aforementioned one developing saturation jumps, Lagrangian models may face challenges in producing physically meaningful solutions. Here, we choose a regularization approach based on artificial diffusion/dissipation, and incorporate an adaptive diffusion coefficient. This coefficient is active only in the vicinity of saturation fronts, as is dictated by its saturation-gradient-dependent scaling, which has been conceptualized in Monga et al. (2022)[3]. Moreover, guided by the vanishing viscosity solution of the 1-D Buckley-Leverett problem, the diffusion coefficient was found to scale with the characteristic speeds of the original hyperbolic system.

We demonstrate that the particle tracking scheme accurately captures sharp saturation profiles in a 1-D Buckley-Leverett reference problem. Subsequently, we analyse the particle-based results in the context of a realistic 2-D fracture network embedded in a permeable matrix. In order to extend the applicability of the proposed regularization approach, isotropic and anisotropic variants of the diffusion coefficient tensor, respectively, are assessed for flow scenarios involving, e.g., gravitational effects and heterogeneity in the matrix. Further application areas include the modeling of physical sub-grid effects, such as dissolution of one phase into the other [Tyagi (2011)][4] and precipitation-dissolution type reactions.

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MS10 / **462**

Void deformation and connecting visualization in asphalt mixture under dynamic water pressure

Authors: Hao Shi[None]; Maja Ruecker[1]; Huining Xu[None]

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Water transport under dynamic vehicle load is the primary causation of asphalt pavement water damage. The dynamic water breaks through the inner voids and destroys the micro-structure of asphalt mixture, and consequently degrades asphalt pavement durability. Understanding the microstructure evolution and void connecting during dynamic water load contributes to the water damage mechanism of asphalt pavement.
This study developed a water seepage device for asphalt mixture and used pulse water pressure to simulate the dynamic water load caused by tire crimping. The pulse sinusoidal water pressure with a frequency of 10Hz and a range from 0 to 0.7 MPa was served. X-ray CT scanning was performed on the dry asphalt mixture and also in-situ seepage asphalt mixture after 3, 8, 15, and 20h water load. A 3D digital void model was developed to analyze the void structure evolution. The translation, volume changing, and connecting in void structure were recognized and analyzed. The 3D water-activated void and water passageway were reconstructed.
The result explained the variation of dynamic flow rate curves by analyzing the microstructure evolution during dynamic water pressure load. The deformation characteristics of voids were addressed and its contribution to water extension was analyzed. The 3D visible water passageway and saturation showed the dynamic water transport process and gave direct evidence of the macro seepage behavior variation.
This study proposes a method to quantify the void deformation in asphalt mixture and explains the macro seepage behavior from the micro aspect. It contributes to understanding the water transport in asphalt pavement and improving its durability.

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Poster / **463**

Stability, deformation and rupture of Janus oligomer enabled self-emulsifying water-in-oil microemulsion droplets

Author: Yuequn Fu[1]

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Microemulsions exist widely in nature, daily life and industrial manufacturing processes, including petroleum production, food processing, drug delivery, new material fabrication, sewage treatment, etc. The mechanical properties of microemulsion droplets and a correlation to their molecular structures are of vital importance to those applications. Despite studies on their physicochemical determinants, there are lots of challenges of exploring the mechanical properties of microemulsions by

experimental studies. Herein, atomistic modelling was utilized to study the stability, deformation, and rupture of Janus oligomer enabled water-in-oil microemulsion droplets, aiming at revealing their intrinsic relationship with Janus oligomer based surfactants and oil structures. The self-emulsifying process from a water, oil and surfactant mixture to a single microemulsion droplet was modulated by the amphiphilicity and structure of the surfactants. Four microemulsion systems with an interfacial thickness in the range of 7.4–17.3 Å were self-assembled to explore the effect of the surfactant on the droplet morphology. By applying counter forces on the water core and the surfactant shell, the mechanical stability of the microemulsion droplets was probed at different ambient temperatures. A strengthening response and a softening regime before and after a temperature-dependent peak force were identified followed by the final rupture. This work demonstrates a practical strategy to precisely tune the mechanical properties of a single microemulsion droplet, which can be applied in the formation, de-emulsification, and design of microemulsions in oil recovery and production, drug delivery and many other applications.

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MS23 / **464**

Imaged-based Study of Fluid Droplet Deformation During Immiscible Ferrofluid Flooding

Authors: Luming Cha[None]; Masa Prodanovic[1]; Matthew Balhoff[2]; Ningyu Wang[None]; Yifei Liu[3]

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Ferrofluid, a stable suspension of superparamagnetic nanoparticles in a liquid carrier, can be manipulated. In an external magnetic field, either constant or evolving, magnetic forces drives the ferrofluid to deform and move, leading to the deformation of the fluid-ferrofluid interface. This has been extensively used in micro-electromechanical systems (MEMS) and here we are motivated to extended these studies to subsurface porous media application, including enhanced oil recovery and environmental remediation. Unlike MEMS devices where non-wetting or non-aqueous phase liquid (NAPL) droplets are typically the ferrofluid to be deformed and manipulated, this is not possible for subsurface applications: oil or NAPL are to be recovered and only aqueous phase could be the ferrofluid. Incidentally, the high-resolution imaging of wetting ferrofluid / non-wetting fluid displacement are very limited.

A converging-diverging single channel glass micromodel with varying depth was fabricated using a standard lithography procedure. The single channel was initially saturated with brine, and then

saturated with a mixture of decane and mineral oil. The micromodel was then flooded using a water-based ferrofluid under a microscope for 47 hours until no noticeable movement of remaining oil droplet was observed and the system was assumed a steady-state. Then, a magnetic field a) transverse to the flow direction and b) rotating magnetic field were applied to the system in separate experiments.

The magnetic field caused oil droplet deformation (specifically, elongation along the magnetic field direction), and dynamic breakup into smaller droplets and subsequent residual oil saturation reduction in a rotating magnetic field. In addition to studying saturation differences, we quantify the curvature of several oil droplets where the resolutions allows before and after the magnetic field application. We finally focus on experiments in a Hele-Shaw cell without flooding, where we observe self-assembly of oil droplets, the formation of the hydrophilic magnetic nanoparticle microstructures (chains under the magnetic field) and their interaction with the oil blobs.

The experimental results show that, during a ferrofluid flooding, in the case of multiple residual fluid droplets within a pore, the fluid droplets can be deformed and potentially controlled using an external magnetic field. Such deformation by the magnetic force can aid or obscure the mobilization of the fluid droplets and has a potential to control the trapped oil saturation near the wellbore in enhanced oil recovery, and to control fluids in MEMS.

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MS13 / **465**

Bound water transport by diffusion in wood-revealed by Nuclear Magnetic Resonance

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Co-authors: Rahima SIDI-BOULENOUAR [2]; Benjamin MAILLET [2]; Philippe COUSSOT [3]

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Wood is extensively applied in various fields such as construction, tooling, sculpture, boat building. The water content within wood plays a crucial role in influencing its performance across different contexts. For example, a large portion of water must be removed from wet or green (fresh cut) wood to mitigate further dimensional variations under varying humidity conditions. In this context, the transport of bound water (absorbed between cellulose microfibrils, up to 30% of the dry mass, and at

the origin of swelling) plays a fundamental role. However, measuring these transport properties is challenging as this bound water is contained in nanopore inclusions. Moreover, it was shown that during standard imbibition there is a strong coupling between bound water and free water [1-2]. Here, for the first time, we develop experimental conditions allowing to prevent most free water (in vessels or fibers) imbibition in hardwood (oak and poplar). We then follow the progression of bound water by NMR relaxometry. This allows to determine in a straightforward way the diffusion coefficient of bound water. The results reveal that the transport diffusion coefficient of bound water in hardwood is rather large, typically in the order of 10-9 m2/s. More precisely, the diffusion in poplar occurs at a faster rate compared to oak samples. Additionally, we show that the fastest rates of diffusion are observed in the longitudinal direction, followed by the radial and the tangential directions. This research underscores the mechanisms and complexity of bound and free water transfer in bio-based materials and provides an insight into the processing and protection of wood.

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Poster / 466

Integrating LUCAS data with AI-driven models for predicting soil Salinization across the EU

Author: Mohammad Aziz Zarif[1]

Co-authors: Amirhossein Hassani [2]; Panos Panagos [3]; Inma Lebron [4]; David A. Robinson [4]; Nima Shokri [1]

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Soil salinization influences vegetation, biodiversity, crop production, land-atmosphere interactions, soil health and ecosystem functioning. Quantifying soil salinity is essential to mitigate its determinantal effects (Hassani et al., 2020; 2021). This study utilizes an AI-driven approach for the quantification of soil salinity in EU using a wide range of environmental covariates including soil properties, terrain attributes, climate, and remotely sensed variables. Soil salinity point data from the LUCAS survey (2015 and 2018) were used for the training and validation of the models. Different algorithms were employed in our analysis including Random Forest, LightGBM, and XGBoost, with XGBoost demonstrating superior accuracy in predicting soil salinity across EU. The predictive model output is a gridded dataset illustrating the spatial and temporal variations of soil salinity, with corresponding uncertainty maps. This work represents one of the first attempts to integrate LUCAS data with AI models, aiming to generate soil salinization maps specifically designed for EU soils. The outcome

will contribute substantially toward devising necessary action plans for protection of EU soils against salinization and degradation which is at the heart of the European Green Deal, Paris Agreement, and the United Nations Sustainable Development Goals especially UN SDG15.

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MS09 / **467**

Combined effect of pore geometry and wettability characteristics on entry capillary pressure

Author: Tongke Zhou[1]

Co-authors: Mehrdad Vasheghani Farahani [2]; Senyou An [3]; Vahid Niasar [4]

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Immiscible two-phase flow in porous media is a universal phenomenon in various natural and industrial processes. Its invasion pattern is determined by the interplay between viscous and capillary forces, neglecting the influence of buoyancy at a small scale. In numerous scenarios in porous media, the capillary forces in drainage process are dominant, which emphasize the importance of precisely computing entry capillary pressure. Existing equations for the calculation of entry capillary pressure, based on the Young-Laplace equation and MS-P method, rely exclusively on cross-sectional geometrical details, and utilize wettability values obtained from flat surfaces to intricate three-dimensional pore structures. However, the effects of three-dimensional pore structures on the curvature of fluid-fluid interface along the flow direction are neglected in these equations.
This work underscores the significance of three-dimensional pore geometry in influencing interface movement and entry capillary pressure, particularly in situations involving intermediate wettability that can introduce complexity to interface behavior. The dynamic evolution of capillary pressure and fluid-fluid interface morphology during two-phase drainage capillary-dominated displacement in both regular capillary tubes and irregular pores extracted from X-ray microtomography images

of real porous media were investigated using the volume-of-fluid (VOF) method. The results indicated that the capillary pressure experiences a temporary decrease, or even becomes negative under intermediate wettability when the interface enters the converging segment as the specified contact angles in a three-dimensional space force the interface to decrease its curvature or even inverse the curvature. This phenomenon is the result of the complex interaction of the solid wall in flow direction, cross sectional geometry normal to the flow and the contact angle. This interesting finding challenges conventional expectations and emphasizes the importance of considering dynamic conditions and wettability effects. The statistical analysis of the interface curvature at the point of maximum capillary pressure revealed the effect of three-dimensional structure on local interface curvature under different wettability conditions. Additionally, the numerical results show that the corner flow becomes unstable under intermediate wettability which leads to less remaining saturation. This study raises doubt on the reliability of existing analytical methods for predicting entry capillary pressure as they overlook the geometrical details along flow direction and lack geometric validity across all range of contact angles. Considering the importance of entry capillary pressure in drainage invasion pattern, it is important to develop models that can improve prediction of entry capillary pressure.

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MS09 / **468**

Measuring (non)stationarity in porous media images and what it means for pore-scale simulations

Authors: Kirill Gerke[1]; Efim Lavrukhin[None]; Andrey Zubov[None]; Marina Karsanina[None]

[1] *RAS*

Corresponding Author: cheshik@yahoo.com

The structures we obtain with, for example, X-ray tomography imaging and then use for pore-scale imaging actually says a lot about the applicability of obtained simulated results. For example, to utilize classical homogenization scheme and obtain continuum scale properties such as permeability, relative permeabilities and numerous others, one needs to establish representativity, which is equal to structural homogeneity of the sample 1. While no natural sample is strictly stationary 2, we shall show that weak stationarity can be effectively established for the purpose of representativity through the analysis of images produced by stationary random processes. But where is that threshold between homogeneous and inhomogeneous structures and why is it important for pore-scale simulations?
The first question highlights the central problem of the blurred interface between heterogeneous and homogeneous, which also depends on the metrics used for its identification. Our results uncover the physics of structural stationarity quantification, based on correlation functions and clustering based on these functions different between image subregions [3]. By applying the methodology to a wide variety of synthetic and real images of binary porous media, we confirmed computationally that

only periodically unit-celled structures and images produced by stationary processes with resolutions close to infinity are strictly stationary. Natural structures without recurring unit cells are only weakly stationary. We established a physically meaningful definition for these stationarity types and their distinction from nonstationarity. In addition, the importance of information content of the chosen metrics is highlighted and discussed [4].
In this presentation we shall focus on:
- Methodology to analyze the porous media images to establish their homogeneity;
- The importance of stationarity to establish REV;
- The crucial role of image analysis with structural metrics prior to any pore-scale simulations.
As we argue, the image analysis based on structural metrics is necessary prior pore-scale simulations. We discuss all the details to establish such an analysis protocol and lay down major methodological procedures.

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Poster / 470

Influence of non-stationarity within porous media sample on its flow properties

Authors: Marina Karsanina[1]; Nickolay Evstigneev[None]; Kirill Gerke[2]

[1] *Schmidt Institute of Physics of the Earth of Russian Academy of Sciences, Moscow, Russia*

[2] *RAS*

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The structure of the sample defines its physical properties. The homogenization based on different fields (e.g., pressure and velocity for permeability property) produces general property of the sample. For this property to be useful for continuum-scale modelling it has to be representative for the

volume it will be substituted for in the next level model. This explains the importance of conventional REV concept. To be a REV, the structure has to be statistically homogeneous 1, but this is not necessarily achieved in real porous media samples such as rocks and soils 2. This is where pore-scale modelling gets really handy –we can still perform homogenization and substitute the averaged property. In this contribution we discuss the influence of spatial non-stationarity on flow properties using full permeability tensor [3,4] as an example. To establish interrelationships, we create artificial porous media structures with different degrees of non-stationarity using stochastic reconstruction methodology [5,6].
In this presentation we shall focus on:
- Methodology to produce porous media structures with different degree of anisotropy;
- Tensorial property assessment for such structures;
- Applications for real homogenization and upscaling cases.
The degree of stationarity of the stochastic reconstructions had a significant influence on the physical properties of the reconstructed binary structures—computed full permeability tensors showed different degree of anisotropy and off-diagonal terms values. The proposed approach to produce non-stationary structures from ensemble averaged set of correlation functions opens numerous ways to attack theoretical and practical problems with natural and artificial porous materials with statistically inhomogeneous structure. Moreover, it is possible to produce large scale inhomogeneous porous structures to parameterize, test and verify different upscaling schemes starting from pore-scale.

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1. Lavrukhin, E. V., Karsanina, M. V., & Gerke, K. M. (2023). Measuring structural nonstationarity: The use of imaging information to quantify homogeneity and inhomogeneity. Physical Review E, 108(6), 064128. 2. Gerke, K. M., & Karsanina, M. V. (2021). How pore structure non-stationarity compromises flow properties representativity (REV) for soil samples: Pore-scale modelling and stationarity analysis. European journal of soil science, 72(2), 527-545. 3. Gerke, K. M., Karsanina, M. V., & Katsman, R. (2019). Calculation of tensorial flow properties on pore level: Exploring the influence of boundary conditions on the permeability of three-dimensional stochastic reconstructions. Physical Review E, 100(5), 053312. 4. Evstigneev, N. M., Ryabkov, O. I., & Gerke, K. M. (2023). Stationary Stokes solver for single-phase flow in porous media: A blastingly fast solution based on Algebraic Multigrid Method using GPU. Advances in Water Resources, 171, 104340. 5. Karsanina, M. V., & Gerke, K. M. (2023). Stochastic (re) constructions of non-stationary material structures: Using ensemble averaged correlation functions and non-uniform phase distributions. Physica A: Statistical Mechanics and its Applications, 611, 128417. 6. Karsanina, M. V., & Gerke, K. M. (2018). Hierarchical optimization: Fast and robust multiscale stochastic reconstructions with rescaled correlation functions. Physical Review Letters, 121(26), 265501.

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MS04 / **471**

Dynamic soil structure imaging experiments and their digital model representation

Authors: Marina Karsanina[1]; Kirill Tolstygin[None]; Andrey Zubov[None]; Dmitry Fomin[None]; Anna Yudina[None]; Konstantin Romanenko[None]; Konstantin Abrosimov[None]; Kirill Gerke[2]

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It is now well recognized that soil structure is dynamic and changes due to numerous reasons, most notably due to saturation changes. In or study, we have sampled 15 soil samples and performed a detailed X-ray microtomography (XCT) imaging study of the full wetting-drying curve 1. By analyzing the XCT images, we revealed the dynamics of soil pore structure under slow water changes. In total, our analysis is based on 135 3D tomography scans (9 soil moisture points for each sample). We were able not only to visualize structural dynamics (which showed significant changes within the soil at ~10 μm –3 mm pore sizes range) but also computed major classical morphological metrics. The analysis of these parameters and conceptual model of structural behavior revealed that after the wetting-drying cycle the studied soil degraded in general. This is contrary to the prevailing previous findings for mainly compacted soils where wetting-drying cycles led to structural improvements. We also found that classical metrics are not able to describe structural changes due to their low information content 2.

Now, we need something reliable to describe all structural changes and create model to describe the changes we observe din the experiments. Such a descriptor to create a digital structural model has to fully describe both geometry and topology of the soil sample and possess high information content. We shall argue that a set of directional correlation functions [3] is enough for this purpose. Compared to classical metrics they 1) contain all classical metrics within them and can also be extended to include topological measures such as persistent diagrams [4]; 2) allow to describe anisotropic structures [5]; 3), have measurable information content 2; 4) if needed, the information content can be augmented with higher number of functions in the set and with higher-order functions [6,7]; 5) allow to establish stationarity and representativity of the structure itself [8,9]; 6) can collect dynamic structural information from different scales [10] –the very aim of the research in this area.

In this presentation we shall focus on:

- Experimental studies of soil structure dynamics by imaging with XCT;
- Description of dynamic soil structure without the use of classical approaches in the form of scalar characteristics;
- Creation of digital model of soil structure dynamics with high information content vector descriptors in the form of correlation functions.

In addition to experimental results and their interpretation, we discuss the major implications of our findings and outline a possibility to deepen our understanding of soil structure-function relationships, including dynamic hydraulic soil properties and 3D soil structure digital model based on correlation functions.

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MS17 / **472**

Pore-scale Simulations On The Impacts Of Hydrate Production Approaches On Gas And Water Transport In Hydrate-bearing Sediments

Author: Zhuoran Li[1]

Co-author: Guan Qin [1]

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OBJECTIVES/SCOPE
Gas and water transport, which is controlled by the pore characteristics and capillarity in hydrate-bearing sediments (HBS), is one of key factors affecting the gas production. Hydrate production approaches (HPA) can significantly influence the dissociation pattern, affecting the pore structures and the transport of fluids. To elucidate the impacts of HPA, a reactive-transport lattice-Boltzmann (LB) model is applied to describe dissociation evolutions. Then, a phase-field LB model is developed to describe the fluids transport.
Methods
To simulate the dissociation evolutions under different HPA, a reactive-transport LB model, which can describe the hydrodynamic process, conjugate heat transfer and chemical reactions, is applied. To simulate the transport of immiscible fluids, which exist obvious density contrasts, a phase-field LB model with the conservative form of interface-tracking equation is developed to suppress the spurious currents at phase interfaces. To describe the fluid-solid interactions, the bounce-back condition is applied for both solid phases (hydrate and grains) to achieve the non-slip condition and the wettability condition is applied for grains and hydrate to describe the wettability behavior.
Results
After the validations for the LB models, the synthetic structures of HBS were applied in our simulations. Two most common HPA, which are called as depressurization (DP) and thermal stimulation (TS) approaches, were respectively considered to stimulate the hydrate dissociation. The dissociation processes were simulated by the reactive-transport LB model to capture the geometric structure evolutions. Then the steady-state relative permeability measurement processes were simulated by the phase-field LB model for two HPA cases under several hydrate saturations (Shyd). The results showed that because of different dissociation patterns under two HPA, the relative permeability of gas in the TS case is obviously larger than that in the DP case at the same Shyd. This indicates that

the TS approach is more conducive to gas production. The reason for this phenomenon is that the void spaces formed in the DP case were dominated by small pores, whereas wide connected paths can be formed in the TS case. In the hydrophilic HBS, water is prone to occupy small pores under capillary pressure, separating the gas and suppressing its transport in the DP case. In the TS case, gas is easily accumulated in connected paths, resulting in higher gas permeability.
Novelty
The phase-filed LB model applied in this study is capable to handle and suppress the spurious currents at phase interfaces, ensuring a satisfactory numerical stability and accuracy. Thus, the real density contrasts between the water and gas under the in-situ thermodynamic conditions can be considered in the simulation. The impacts of HPA on the gas and water transport were quantitively analyzed by simulating multiphase flow processes in HBS.

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MS11 / 473

Assessing pH Impact on Miscible Phase Displacement and Mixing within Porous Structures

Author: Tongzhou GAN[None]

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pH-induced reactive transport among miscible phases in porous environments is pivotal in carbon capture and storage (CCS) applications, especially in the carbon sequestration process, where the mixing process among the miscible phases affects the pH transport. However, separating the mixing from the pH migration is challenging due to the pore-scale heterogeneities and limited understanding of the role of pH in the mixing and displacement processes within porous media.. In this study, we use two sets of basic water solution to displace weak acidic water glycerol mixed solution, one set with certain concentration of pH-sensitive fluorescent dye Pyranine as the pH indicator in both phases to examine the influence of pH on miscible phase flow and displacement in porous media, the other set with fluorescent dye Rhodamine 6G as the mixing process indicator, explicitly visualizing how heterogeneity affect the mixing and displacement patterns and comparing this theoretical pH pattern obtained from the mixing process with the actual visualized pH migration pattern. The research employs confocal microscopy to visualize these processes, revealing diverse patterns across different heterogeneity porous media types, and mainly illustrates the significant role of pH in shaping fluid dynamics and reactive transport by leading to enhanced fluid migration and mixing. An initial outcome has showed that the migration of pH follows a different mechanism from the mixing process. Thus, it offers new insights for modeling such complex systems in natural and industrial

settings, which may be practical for field-scale applications by outlining the details of pore-scale transport and reaction

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MS06-A / 474

Experimental investigation of capillary effects on solid-liquid interactions in porous media at the decimetric column scale

Authors: Meysam Golmohammadi[1]; Lionel Mercury[2]; Stéphane Gaboreau[3]

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The capillary state of water in porous media is of paramount importance at the caprock-aquifer interface to prevent any CO2 leakage. But it also significantly influences gas dissolution and solid mineralization reactions, crucial for CO2 trapping and earth science engineering. Capillarity-based geochemistry has been experimentally documented and quantified at the one-pore sale. Yet, capillary water exerts super-solubilizing effects on solids and gases 1, induces cold boiling, and modifies the stress field within the host matrix 2. These effects must now be established experimentally at the upper core scale. At this thousands of pores scale, the effect(s) of capillarity competes with the dry conditions intrinsic to unsaturated media that limits the water availability, and with the evolution of the reactive surface area which depends on the liquid/air distribution and the passivation of solid surfaces through secondary phase precipitation. We are discussing the experimental design and first results to help unravel this interwoven sketch, which is much needed for accurate predictions in any long-term scenarios of aquifer-air 'tandem'technique (CO2 storage, nuclear wastes tunnels, energy storage, ⋯).

In this study, we examine the brucite (Mg(OH)2) carbonation in unsaturated columns flushed with a CO2 gas flow. The design varied from one experiment to the others by the initial water content, the gas flushing composition, the gas flow rate, and the granulometry of the column materials. These experiments provide simplified models for comprehending carbon mineralization reactions in partially water-saturated porous media, resembling conditions in unsaturated zones of natural systems or disturbed and industrial settings. The main goal of our investigation is to evaluate how capillary water impacts the precipitation of hydrous Mg-carbonates.

Experiments are performed in decimetric unsaturated columns filled with brucite grains and quartz sand (Figure 1). Capillary conditions are established by flushing the column with N2 air at low relative humidity (RH) illustrated below for one dataset (Stage 0, RH 50%, Figure 2). After stabilization, the gas composition is turned to CO2-H2O, initiating carbonation (hydromagnesite formation) by pore-scale interaction between CO2, liquid water, and brucite. The column mass variation shows a first decreasing stage linked to the evaporation of 15% of the initial water, before reaching a plateau, and then displaying an increasing stage related to the carbonation reaction. The CO2 breakthrough curve reveals three distinct stages (Figure 2). Stage 1 exhibits minimal CO2 at the column outlet, primarily due to bulk brucite carbonation. In Stage 2, a decline in reactive brucite abundance slowdowns the carbonation rate, leading to an increase in CO2 content in the effluent gas. Finally, Stage 3 demonstrates a CO2 concentration aligning with the supplied gas composition, signifying the cessation of the carbonation reaction. This is also evident by the stability of the column weight at this stage.

In summary, the evaporation process and the carbonation reaction occurring in an extended pore network at the column scale both appear sensitive to the capillary conditions in porous media which can grow and express oneself depending on various factors that will be discussed in this contribution.

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1 C. Hulin and L. Mercury, “Capillarity-driven supersolubility in dual-porosity systems,”Geochim Cosmochim Acta, vol. 252, pp. 144–158, May 2019, doi: 10.1016/J.GCA.2019.02.026. 2 L. Mercury et al., “Quartz Stressing and Fracturing by Pore Pressure Dropping down to Negative Pressure,”ACS Earth Space Chem, vol. 5, no. 2, pp. 170–185, Feb. 2021, doi: 10.1021/ACSEARTHSPACECHEM.0C00224/ASSET/IMAGES/MEDIUM/SP0C

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MS06-A / 475

Impact of wetting films on stability diagrams of two-phase flow in porous media

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The stability of two-phase flow in porous media is known to depend on the viscosity ratio and on the capillary number. The transition from a stable regime, to viscous or capillary fingering is not always clear. In this work, we investigate the role of wetting films on the stability of two-phase flow during a drainage. Such films are ubiquitous in porous media and appear when the solid is strongly wetted by one of the fluid. We develop a new dynamic pore-doublet approach combined

with microfluidic experiments to highlight the role of the wetting films on the stability diagrams. We demonstrate that the layers of wetting fluid along the solid walls significantly alter the stability of the invasion.

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MS17 / **476**

Pore-scale modelling of non-linear rock deformation under low-stress ranges

Author: Rui Li[None]

Co-authors: Yi Yang [1]; Yuxuan Zhang [1]; Wenbo Zhan [1]; Jianhui Yang [1]; Yingfang Zhou [1]

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Under increasing compressive stress, intrinsic micro cracks and pores in rock samples close, leading to non-linear deformation at low-stress ranges. This intrinsic non-linearity significantly affects rock geophysical properties under confinement, such as rock stiffness and transport properties. Many studies have reported this low-stress inelastic behaviour in experiments, and some analytical models have been established to predict this phenomenon. However, in the perspective of pore-scale numerical modelling, this non-linear deformation was completely ignored, and the rock was treated as elastic in simulations until rock failure. As a result, the modelled rock geophysical properties in the non-linear part are quite different from the experimental results. To address this issue, we proposed a method to predict the rock geophysical properties at the low-stress non-linear range through numerical simulations. A crucial aspect of this approach involves dividing the transition phase between macro pores and the solid phase into several sub-phases with varying porosities, all treated with zero elastic moduli. These sub-phases deform and transition to other phases based on the extent of deformation under the applied strain conditions in the Finite-Element method. The ability to interchange between different phases in the rock model enables the modelling of non-linear behaviour within the low-stress range. We validated this method on various rock samples, and the results align well with experimental measurements.

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Research on fracturing monitoring method based on deep learning

Author: Yueying Wang[None]

Co-authors: Aimin Lv ; Jun Yao

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In view of the advantages of paramagnetic particles, such as environmental properties, filling perfectly the effective fracture space and unlimited detection time, it is expected to be an important method of fracturing real-time dynamic monitoring that the magnetic fracture monitoring using paramagnetic particles. Rapid and accurate inversion of fracture geometry is the core and key of real-time dynamic monitoring, which directly affects the implementation time and fracturing quality. Inversion of fracture geometry based on magnetic anomalies is a typical inverse problem. In this paper, a data-driven deep learning method is adopted to establish the nonlinear relationship between spatial magnetic anomalies (magnetic anomalies caused by paramagnetic particles under the action of external magnetic fields) and magnetic objects (fractured fractures filled with paramagnetic particles) through the training and learning of UNet models. To realize the rapid inversion imaging of fractures by magnetic method in the process of artificial fracturing.
The development of computer hardware and various open source frameworks have enabled the rapid application of Deep Learning methods in various fields which have achieved great progress. In this paper, we predict the location and shape of the fractures according to the magnetic susceptibility based on UNet model. It contains training and testing procedure. At first, we acquire the correspondence between the spatial magnetic anomalies and the magnetic objects during training, and then using the trained UNet model, take the magnetic anomalies data as input and magnetic susceptibility as output. Compared with the other methods, such as microseismic, geostress analysis and so on, using the Deep Learning Method to predict the fractures has the following advantages: predicting rapidly and saving a lot of time, driven by the data and no human influence, testing time no limit, obtaining the better imaging results. This method applies deep learning to real-time dynamic monitoring of fracturing fractures, improves the speed and accuracy of fracture inversion imaging, and enhances the practicability of magnetic dynamic monitoring method.

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Poster / 480

Computational and Topological Methods for In-situ Characterisation of Hetrogeneous Surface Wettability in Porous Media

Author: Ying Da Wang[1]

Co-authors: Chenhao Sun ; Kunning Tang [1]; Luke Kearney [2]; Martin Blunt [3]; Peyman Mostaghimi ; Ryan Armstrong

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The efficiency of nano- and micro-porous materials in absorbing and releasing fluids, like CO_2 in geo-storage or water and gas in fuel cells and electrolyzers, depends on their surface wettability. Measuring wettability accurately is complex due to varying dynamic forces, chemical diversity, and surface texture. In situ measurements, which could assess wettability as a local contact angle (the angle at which a denser phase like water meets a solid in the presence of another phase like hydrogen, air, or CO_2), face challenges in precisely determining fluid curvatures, contact points, and the loops formed by multiphase fluids. We introduce a new, advanced topological method for in situ contact angle measurement and conduct a comparative analysis of existing geometric and topological techniques, evaluating their precision on ideal surfaces, CO_2-containing porous rocks, and water in gas diffusion layers. This novel approach offers more accurate and reliable in situ measurements for uniformly wetting environments compared to past topological methods, whereas geometric methods excel in mixed-wetting areas. Additionally, this research includes a detailed open-source platform for in situ wettability assessment in porous materials, which has significant implications for gas geo-storage, fuel cells, electrolyzers, filtration, and catalysis.

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Poster / 482

Study on the Emulsification Characteristics of Heavy Oil during Chemical Flooding

Authors: Jianbin Liu[1]; Shun Liu[1]; Xin Chen[1]

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Chemical flooding is a very important method to the efficient development of heavy oil reservoir. A clear understanding of the relationship between emulsification characteristics of heavy oil during chemical flooding and test methods that current used to evaluate the properties of chemical flooding agent can be useful for oilfields development of the heavy oil. In this study, the oil-water interfacial tension (IFT) and oil in water (O/W) emulsion properties (emulsification state, droplet size, viscoelasticity and stability) formed by six chemical flooding agents at different concentration are tested. Then, combined with the heavy oil flooding dynamics, the emulsification characteristics of heavy oil during the chemical flooding process of are studied and the influence mechanisms of O/W emulsion on oil recovery are clarified. Finally, the emulsification effect of heavy oil on injection profile turnover is studied by parallel sand-packed tube experiments. Studies show that all six chemical flooding agents can greatly reduce the IFT of heavy oil-water (more than 90%). However, the stronger the emulsification ability, the smaller the droplet size, the better the viscoelasticity and the stronger the stability of O/W emulsion, the better heavy oil recovery of the chemical flooding agent. This is mainly because the most effective action stage is the time it takes from the chemical flooding agent injected to the O/W emulsion front reach the production outlet. During this period, the amount of emulsified heavy oil, the width of emulsification zone and the properties of formed O/W emulsion all affect the heavy oil flooding efficiency. Therefore, when screening chemical flooding agents, the emulsification speed, the droplet size and the viscoelasticity of formed O/W emulsion are the primary evaluation factors. In addition, through the parallel sand-packed tube experiment, it is found that the stronger the emulsification ability of chemical flooding agent, the better the performance of formed O/W emulsion, the stronger the profile turn over ability. For reservoirs that water flow channel has formed, using profile control agents to effectively block dominant flow channels can improve the emulsification ability of chemical flooding agents, thus achieving the purpose of improving the swept area. The research results can provide guidance for the screening of chemical flooding agent with emulsify character and construction process optimizing in heavy oil reservoirs development.

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Poster / **484**

An efficient numerical simulation of coupled thermo-hydro-mechanical processes in deep tight gas reservoirs

Authors: Yongliang Tang[1]; Yu-Shu Wu[2]; Zhaoqin Huang[3]; Jun Yao[None]

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Deep tight gas is an important unconventional natural gas resource, and it is an important target of exploration and development in recent years. Deep tight gas reservoirs are high-temperature, high-pressure, and high-stress with complex gas–water relationships, and its occurrence and flow mechanisms are still unclear, making the simulation of deep tight gas reservoirs still a challenging problem. Aiming at the key problems faced in the development of deep tight gas reservoirs, this paper establishes a flow-stress-temperature field coupled mathematical model and numerical model, studies the thermo-hydro-mechanical sequential decoupling method to solve the coupled mathematical model, and forms a multi-field coupled simulation technology which provides theoretical support for the development of deep tight gas. Based on the thermo-hydro-mechanical coupling calculation module, this paper conducts research on the influence of thermo-hydro-mechanical multi-field coupling parameters on the production and development performance, and it further verifies the practicability of our proposed model in real
reservoirs.

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MS17 / **485**

Mineral composition and concrete gradation of sandy clay on CO2 hydrates formation

Author: Jianzhong Zhao[1]

Co-authors: Chi Zhang [1]; Qiang Gao [2]; Yue Ma [1]

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Sandy clay is the main porous medium for the occurrence of gas hydrates in nature. Hydrate-based technology for CO2 sequestration in marine and permafrost layers is a promising and potential technique. To investigate the influence of formation properties on CO2 sequestration, experiments were conducted under an initial pressure of 5.5 MPa and temperature of 1.27 ℃. The influence of different

mineral compositions and concrete gradation of sandy clay for CO2 hydrate formation were analyzed. The pressure-temperature changes, CO2 hydrate average formation rate, CO2 consumption, and phase saturation were calculated during the CO2 hydrate formation process. The results show that the CO2 hydrate average formation rate decelerated with the increase of coarse sand proportion due to the reduction of specific surface area, and the CO2 hydrate average formation rate is the smallest when the ratio of fine-grained sand to coarse-grained sand particle sizes (mass ratio of each component, the same below) is 1.0: 2.0, which is 12.60 mmol/min. Montmorillonite is not conducive to CO2 hydrate formation; the CO2 hydrate average formation rate of the sand group (contains fine-grained sand and coarse-grained sand) is higher than that of the sandy clay group (contains fine-grained sand and montmorillonite clay). The experiments in the sand group are more likely to achieve high hydrate saturation and CO2 consumption, making it more suitable for CO2 sequestration in areas with mineral compositions containing fine-grained sand and coarse-grained sand. The CO2 consumption rates for the ratio of fine-grained sand to coarse-grained sand and clay mineral particle sizes of 1.0: 0.5 are 0.86 mol and 0.77 mol, respectively. With the increase in the proportion of coarse-grained sand and clay minerals, both the hydrate saturation and CO2 consumption gradually decrease. The ratio of fine-grained sand to coarse-grained sand and clay mineral particle sizes of 1.0:0.5 is suitable for CO2 sequestration using the hydrate-based technology.

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MS08 / **487**

Probing Transport in Geologic Porous Materials by Fast X-ray Micro-Computed Tomography

Author: Takeshi Kurotori[1]

Co-author: Ronny Pini [1]

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Understanding the time evolution of solute transport at the pore scale in geologic porous media is crucial in many subsurface engineering applications, including underground gas (e.g. H2 and CO2) storage. While transport processes in rocks can be investigated by dynamic 4D imaging, such as X-ray and neutron-based computed tomography, most of the observations so far have been limited to the continuum scale (image resolution approx. 1 mm and above). These observations have improved our understanding of non-Fickian transport in rocks 1. Yet, the lack of spatial resolution of these methods precludes the unambiguous interpretation of the transport mechanisms at play, because the relevant mixing processes initiate at the pore scale. Recent advances involve the uses of fast X-ray micro-computed tomography (fast μCT), which allows direct micron-scale imaging of fluid transport at a time resolution on the order of tens of seconds.

Here, we analyse a comprehensive data set of 4D imagery acquired by fast μCT available on the Digital Rocks Portal [2,3]. The dataset consists of dynamic images of solute transport during miscible displacement in three porous media (diameter: 6 mm, and lengths: 16 or 20 mm), namely sintered beadpack, Bentherimer sandstone, and Savonnières limestone. Tracer tests were performed at various Péclet numbers, covering the range Pe = 2 –20. In each test, fast μCT scans were continuously acquired at the sample inlet with the field of view of 8.8 (H) x 8.8 (W) x 5.0 (L) mm, and at spatial and time resolutions of 14 μm and 12 s, respectively. We have analysed this rich dataset by applying the concept of residence time (RT) at different length-scales and by considering its spatial variability within the sample. Specifically, we computed RT curves for individual pore volume elements (PVE) in the sample (> 100 curves) and identified variations with both size and spatial location of the PVE. The strength of pore-scale heterogeneity is thus quantified by comparing the experimental RT with the theoretical counterparts. To quantify the degree of non-uniformity of the concentration field, we also examined the extent of mixing within individual PVE using various metrics, including the dilution index, the intensity of segregation and the spreading length.

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1 Pini, R., Vandehey, N.T., Druhan, J., O'Neil, J.P. & Benson, S.M. Quantifying solute spreading and mixing in reservoir rocks using 3-D PET imaging. Journal of Fluid Mechanics, https://doi.org/10.1017/jfm.2016.262 (2016). 2 Van Offenwert, S., Bultreys, T. & Cnudde, V. Saturated solute transport micro-CT dataset in sintered glass and Bentheimer sandstone. Digital Rocks Portal, https://doi.org/10.17612/5ww0-gh34 (2019). [3] Van Offenwert, S., Bultreys, T., Boone, M. & Cnudde, V. Saturated solute transport micro-CT dataset in Savonnières limestone. Digital Rocks Portal, https://doi.org/10.17612/ypvb-jg13 (2020).

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MS06-B / 491

Interfacial tension reduction mechanism by nanoparticles at heavy oil-carbonized water interface from molecular dynamics approaches

Author: Xiaofei Sun[1]

Co-authors: Guo Yu [1]; Haoyu Ning [1]; Zixiong Jia [1]; Guanglei Xie [1]; Yongbin Zhao [1]; Xinyu Sun [1]

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Nanoparticle-enhanced carbonated water (NP-enhanced CW) is a novel and promising injection agent for coupled enhanced heavy oil (HO) recovery and CO2 storage. The main objective of this study is to investigate the interfacial tension reduction mechanism by nanoparticles (NPs) at HO-CW interface from molecular dynamics approaches. The influences of NPs on the Interfacial tension of HO-CW systems under reservoir conditions were studied. In addition, the influences of NP type, NP concentration, CO2 concentration, pressure, and temperature were investigated and the enhanced

oil recovery mechanisms of nanoparticle-enhanced CW were also discussed. The results revealed that the ability of the five NPs to reduce the IFT of the HO-CW systems was as follows: SiO2 NPs > Al2O3 NPs > TiO2 NPs > Fe NPs > CuO NPs. The interfacial tension value of the HO-CW system decreased by 39.69 % due to the presence of SiO2 NPs. An optimal NP concentration existed to decrease the interfacial tension of the HO-CW systems. The interfacial tension values of the HO-CW systems in the presence of SiO2 NPs decreased with increasing the CO2 concentration, temperature, and pressure. This study is helpful in deeply understanding the microscopic mechanisms of NPs affecting the interfacial tension of HO-CW systems during the injection processes of NP-enhanced CW. The results also provide a valuable reference for the injection of the NP-enhanced CW as a new technology to enhance HO recovery and underground storage of CO2.

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MS17 / 492

Coupled Thermal-Hydraulic-Mechanical-Chemical Simulation for Underground Coal Gasification

Authors: Zhuocheng Hu[1]; Jun Yao[2]; Hai Sun[1]

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China, as the world's foremost consumer and producer of coal, portrays an energy landscape marked by an abundance of coal, a scarcity of oil, and a limited presence of natural gas. The collective coal consumption exceeds half of the global total, and there is an expectation that coal will continue to play a predominant role in the energy paradigm for an extended future period. However, a significant portion of China's coal reserves is situated in deep strata, presenting formidable challenges arising from intricate geological conditions. Consequently, the imperative to innovate advanced technologies for the clean and efficient extraction of coal, particularly from deep seams, becomes paramount.

Underground Coal Gasification (UCG) emerges as a viable, sustainable approach for exploiting these deep-seam coal deposits. This intricate process involves multifaceted elements such as heat transfer, fluid dynamics, mechanics, and chemical reactions, posing significant complexities for effective management. While the UCG in deep seams primarily relies on injection and production controls, the lack of transparency hampers the identification of optimal operational parameters. Addressing these intricacies necessitates the development of a comprehensive numerical simulation model that integrates mechanical, fluid, chemical, and thermal dynamics. In this research, we introduce a Thermal-Hydraulic-Mechanical-Chemical (THMC) model employing sequential coupling, further enriched by an interface code linking the reservoir simulator with the geomechanics module. A pivotal component of our investigation centers on discerning the influence of geomechanics on porosity and permeability during the UCG process, alongside evaluating stress distribution within the cavity

to assess potential risks of spalling and collapse.
The results elucidate that, during UCG, coal undergoes heating and decomposition, resulting in the formation of coal char. The interaction between the char and the gasification agent initiates a multifaceted chemical reaction, yielding gases such as CO, CO2, H2, CH4, among others. Notably, the temperature within the coal seam can reach a peak of 1500℃, giving rise to the development of a semi-circular cavity. Intriguingly, the boundary of this cavity coincides with the region exhibiting the highest concentration of CO2. It is observed that as the injection pressure and flow rate of the gasification agent increase, there is a corresponding rise in the amount of syngas calorific value and CO2, along with the amount of coal processed per unit time. However, this increase ultimately diminishes the energy conversion efficiency of coal gasification. The composition of the gasification agent emerges as a pivotal factor in the UCG process. For example, water has the capacity to augment the rate of coal consumption, promote CH4 production, and elevate the calorific value of the syngas. Nevertheless, an excess of water can lead to a reduction in operational temperature, impeding the generation of high-calorific syngas. Furthermore, the presence of CO2 in the gasification agent can augment CO production without adversely affecting the properties of the syngas. In the upper reaches of the cavity, stress concentrations are discernible, with shear stresses registering several times higher than their initial levels. This phenomenon induces deformation around the cavity.

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Poster / 493

Flow simulation of pore-scale deep shale gas under nano-confinement conditions

Authors: Chaoyang Zhao[1]; Yongfei Yang[2]

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Deep shale gas will become an important part of supporting the growth of China ‘s natural gas production. Compared with the middle shale and shallow shale, the properties and porous flow laws of deep shale gas are more complex. The nano-confinement effects such as adsorption and slippage cannot be ignored in the study of porous flow mechanism of deep shale gas. When the porous flow law of deep shale gas on the pore scale, the influence of nano-confinement effect on the porous flow law needs to be further clarified. In this work, a pore network model containing water-wet inorganic pore throats and gas-wet organic pore throats is established, which conforms to the pore structure characteristics of shale in actual depth. And the permeability of shale gas under different wettability, slippage, adsorption and surface diffusion is studied. Viscous flow, Knudsen diffusion, adsorption, slippage and surface diffusion are considered in organic pores, viscous flow and Knudsen diffusion

are considered in inorganic pores. Different TOC contents are set to study the influence of nano-confinement effect on deep shale gas flow and the flow law of shale gas. The results show that the porous flow of deep shale gas is greatly affected by adsorption and slippage. The surface diffusion of adsorbed gas in organic pores provides more flux for the flow of deep shale gas. When the TOC content is high, the flow of shale gas is mainly controlled by organic pores.

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Study on microscopic oil production characteristics under mixed wetting conditions of shale based on pore network modelling

Authors: Ke Wang[1]; Hai Sun[1]; Xinyi Zhao[1]; Qian Sang[1]; Xueqiang Guo[1]; Mingzhe Dong[2]

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Shale is composed of various mineral components: quartz, feldspar, clay, carbonate, organic matter, etc. The imaging technology with nanometer resolution has observed nanometer-scale pore structures in various components. The shale nanoporous system has strong heterogeneity. The pore size in organic matter and clay is generally smaller than that of quartz pores. What's more, organic matter and inorganic matter show different fluid-solid interactions. It is commonly believed that the organic matter has a strong affinity to hydrocarbon molecules, which leads to oil-wet organic pores, and the inorganic materials are attractive to the water, making the inorganic pores wetted by water. In the process of hydraulic fracturing, a large amount of water-based fracturing fluids imbibes into the matrix under high pressure to drive out oil. The nanometer-scale pores of shale matrix have high capillary forces, which has significant effects on oil/water two-phase flow. The flow and storage characteristics of oil and water in this nanoporous system under mixed wetting conditions are poorly understood. In this study, we established a multi-component pore-scale model containing quartz, clay, and organic matter based on pore network modeling, which reproduces the structural characteristics of various pore systems. A two-phase flow simulation method considering capillary force and viscous force was developed and used to simulate the process of water flooding in the multi-component model. We tracked the dynamic movement of the oil-water interfaces, and obtained the distribution of oil and water in different types of pores. The results show that organic matter has a retarding effect on the water flooding process, with higher organic matter content leading to higher remaining oil saturation. Larger organic pore size and weaker oil-wet of organic matter is beneficial for the mobilization of oil in organic matter. The increase of clay content reduces the displacement efficiency of quartz and clay pores. The results of this study help in understanding the flow behavior of oil and water in shale nanoporous system with multiple mineral components.

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Poster / 496

Experimental and theoretical study of unsaturated flow in fractured media

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Unsaturated flow in fractured media is an important process with relevance to a large number of industrial and environmental application. In this work, we report recent experimental and theoretical investigations on unsaturated flow in single fractures, fracture intersections, and fracture networks. Wo focus on how small-scale flow physics influences the spatial and temporal characteristics of unsaturated flow in discrete fracture networks. We propose theoretical models for predicting water splitting at fracture intersections and for predicting water breakthrough time in an unsaturated fracture network. We validate these models by comparing with experimental observations. We show that the breakthrough time in a fracture network decreases with the increase of initial saturation. We also find that avalanche infiltration mode, i.e., sudden release of a large amount of water from the network, emerges spontaneously in the network, and is modulated by the local splitting behavior. We further show that the power spectral density of the water saturation time series in the network follows a power law with an exponent of −2 for all simulations with different structural parameters and local flow rules, suggesting a universal self-organized criticality behavior for unsaturated flow in fractured rocks.

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Poster / **498**

Assessing the Representativeness and Precision of Three-Dimensional Digital Rock Modeling: A Case Study on Tight Sandstone

Authors: Fei Xian[1]; Min Li[1]; Zizeng Li[1]; Jiamin Hu[1]; Chenyu Li[1]; Xuefeng Liu[1]

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Tight sandstones are characterized by low porosity and permeability, high clay content. Measuring the rock physics properties under low water saturation conditions using the displacement method poses significant challenges. Digital rock physics (DRP) has been emerged as a valueble method for studying of rock physics of unconventional reservoir. It should be noted that the resolution of X-ray Computer Tomography (CT) scans and sample size can impose mutual restrictions. In order to enhance the applicability of rock physics numerical simulation results, it is crucial to adequately assess the representativeness and accuracy of three-dimensional digital rocks. In this study,3 sandstone samples with porosities of 17.0%,10.8%, and 8.4%, and permeabilities of 339.7,13.2, and 0.94 mD, were selected to construct digital rocks. Seven sub-samples with diameters of 25.4,9,7,5,3,2, and 1mm were prepared for each sample. We utilized X-ray CT scanning to generate three-dimensional grayscale images of the samples, with resolutions ranging from 13.5μm to 1.1μm. These images were then segmented into five components- pores, clay, feldspathic, potassium feldspar, and high-density minerals- using a machine learning image segmentation algorithm. The volume content of the principal minerals in the multi-mineral component digital rocks was calculated and compared with the XRD measurement to assess the representativeness of the three-dimensional digital rocks with different size. The porosities of the digital rocks were determined and compared with the porosity measured in lab. This comparative analysis was conducted to evaluate the precision of the digital rocks. The outcomes of three-dimensional digital rock modeling for tight sandstones reveal that three-dimensional grayscale image acquire via CT scanning for the sample with the diameter of 25.4 mm exhibits difficulty in distinguishing between pore spaces and primary mineral types. By considering the composition of randomly distributed high-density minerals as a metric for assessing representativeness, it was found that the variability of this mineral component increases when the sample diameter is less than 5 mm. This suggests that samples smaller than this size may not adequately capture the macroscopic physical properties. As the sample size decreases, the porosity identified in the digital rock increases. However, it consistently remains lower than the experimentally measured porosity, even in the highest resolution 1 mm sample. When accounting for micropores that are smaller than the scanning resolution of CT, and incorporating them into the multi-mineral digital rocks, the computed porosities agree well with those measured in lab.

Keywords：Tight Sandstone, Machine Learning, Digital Rock Physics, Multi-mineral 3D Modeling, X-ray CT Scanning.

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Poster / 499

Constructing Three-Dimensional Digital Rock of Continental Shale with Multi-Mineral Components Using Machine Learning Segmentation Algorithms

Authors: Min Li[1]; Fei Xian[1]; Zizeng Li[1]; Jiamin Hu[1]; Chenyu Li[1]; Xuefeng Liu[1]

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Continental shales are characterized by their highly developed laminations and a high clay content, which pose significant challenges in terms of sample preparation and fluid saturation process for traditional rock physics experiments. Digital rock physics (DRP) has been emerged as an alternative method for unconventional reservoir. The establishment of a high-precision three-dimensional digital rock is crucial to ensure the accuracy of numerical simulations for determining rock physics properties. While continental shale reservoirs exhibit numerous nanopores, indistinct clay particle boundaries, and small fractures in bedding planes, which pose challenges to the segmentation of two or three dimensional grayscale images.X-ray Computer Tomography (CT), Scanning Electron Microscope Mineral Quantitative Evaluation (QEMSCAN), and Multi-spectral Automated Petrographic System (MAPS) tests are performed sequentially on continental shale samples. The scanning resolutions for these tests are 1.35μm, 1μm, and 10nm, respectively. Initially, the grayscale ranges for different mineral components were identified by combining QEMSCAN with CT scans images. Afterwards, a machine learning image segmentation algorithm was employed to partition the CT scan grayscale images into five components: pores, organic matter, clay minerals, feldspathic minerals, carbonate minerals, and pyrite. Subsequently, the same machine learning segmentation algorithm was applied to the two-dimensional MAPS images of the shale sample. This was done to identify pore spaces that were smaller than the CT resolution present in the carbonate minerals, organic matter, and clay minerals, and to calculate the surface porosity.The segmentation results of the X-ray CT scan images indicate that the machine learning segmentation algorithm improve the accuracy in identifying the boundaries of the matrix and pores compared to traditional grayscale-based segmentation method. The machine learning-based image segmentation algorithms can also accurately identify unidirectionally extended microcracks. The contents of the main mineral components calculated from digital rocks agree well with those measured by X-ray Diffraction (XRD). However, the porosity identified in CT images was considerably lower than helium porosity of the samples because only large intergranular pores and fractures can be resolved by CT. There are lots of sub-resolution pores in continental pores as illustrated in MAPS images compared to marine shale gas reservoirs, the organic matter pores in continental shale oil reservoirs are not well developed, and the microporosity is about 5%. The intercrystalline pores in clay minerals are the main reservoir space for continental shale oil, with a microporosity of 10%. The total porosities of the multi-mineral component digital rocks were calculated by considering the volume fractions of the main minerals and their corresponding microporosities. The porosity values obtained from the digital rocks exhibit excellent correlation with those derived from laboratory measurements. The three-dimensional digital rock model serves as a precise representation of the pore structure, enabling quantitative analysis of the microstructure and numerical simulation of the physical properties of continental shale.

Key words: Digital Rock Physics, Continental Shale, Machine Learning Image Segmentation, Pore Structure Characterization, X-ray Computer Tomography (CT) scans Imaging

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Poster / 501

Large PV carbon dioxide flooding mechanism of ultra-low permeability tight reservoir in Songliao Basin

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Corresponding Author: xr1169924518@163.com

Abstract: Based on sandstone reservoir samples in Songliao Basin, carbon dioxide displacement of saturated crude oil core experiments were carried out, combined with nuclear magnetic resonance and oil component analysis, to study the mechanism of carbon dioxide oil recovery. The rock samples with proper permeability including medium permeability, low permeability, ultra-low permeability and tight permeability in Songliao Basin were selected to analyze the effect of permeability on carbon dioxide displacement. The displacement experiment was divided into three stages to analyze the effect of injected PV number on CO2 displacement. Taking large PV carbon dioxide flooding of ultra-low and tight permeability rock samples as the research focus, the mechanism of large PV carbon dioxide flooding of ultra-low permeability and dense reservoirs in Songliao Basin is studied by using the method of controlling variables. Experiments show that large PV CO2 flooding can obtain good recovery results for ultra-low permeability and dense reservoirs. After low-PV displacement, the average harvesting degree of low-permeability and medium-permeability samples was 30.56%, and that of ultra-low-permeability and dense samples was 26.21%. After large-PV displacement, the average recovery degree of low-permeability and medium-permeability samples was 55.92%, and the average recovery degree of ultra-low-permeability and dense samples was 67.00%. This indicates that large PV carbon dioxide flooding can effectively improve reservoir recovery, and the improvement range is more obvious for ultra-low permeability and dense reservoirs. Large PV complete miscible CO2 displacement can obtain a good final recovery degree, up to 67.49%. Complete miscible displacement can well displace various components of crude oil including heavy components. There is little difference in the oil family components in different displacement stages, but there is still an obvious effect of extracting light components. The peak value of oil components gradually shifts from near C12 in the early stage to near C17 in the late stage. The carbon dioxide extraction will make the heavy components of crude oil deposited on the pore throat surface. The deposition phenomenon is more obvious in ultra-low permeability and dense reservoirs when injected with low PV number, while the deposition phenomenon is weak in medium and low permeability oil reservoirs. After large PV carbon dioxide flooding, heavy components in ultra-low permeability and dense reservoirs are well recovered, and the final recovery degree of heavy components is similar to that of medium and low permeability oil reservoirs, indicating that large PV carbon dioxide flooding is more suitable

for ultra-low permeability and dense reservoirs.
Key Words: sandstone reservoir ; carbon dioxide ; ultra-low permeability and dense ; nuclear magnetic resonance (NMR) ; component analysis

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Poster / 503

Density-Dependent Dynamics of Fines Retention and Pore Clogging in Rock Formations: A CFD-DEM Approach

Author: Shitao Liu[None]

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In the realm of geosciences, the phenomenon of fines migration and subsequent clogging in rock formations presents a complex challenge. This process can occur even when fines are smaller than a specific threshold size, known as the critical throat diameter. The dynamics of pore clogging involve interactions on multiple scales - ranging from the transport at the pore level to the mechanical and hydraulic behaviors at the colloid level, down to the electrochemical interplays at sub-colloid scales. Traditionally, the Colloid Filtration Theory (CFT) has been the go-to model, focusing on predicting how colloidal particles are retained under the assumption of clean bed conditions. This overlooks the significant impact of particle aggregation and clogging at the throat passages. While experimental measurements are ideal for assessing filtration efficiency, they fall short in directly examining the intricate movements and paths of particles at the pore level, especially due to the opaque nature of the media involved. Numerical models addressing the full scope of forces in pore clogging have been limited to two-dimensional simulations of rock structures. This research advances the field by employing a combined fines tracking method that integrates Computational Fluid Dynamics (CFD) with a Discrete Element Model (DEM). The approach is designed to predict the retention and clogging of fines, factoring in surface forces and the impact of gravity forces due to density variations between the fines and the saturating brine.

To accurately represent the complex pore structures and simulate particle movement within the rocks, we use a three-dimensional X-ray computed microtomography image of Bentheimer sandstone. An innovative feature of our method is the use of a dynamically adaptive CFD mesh, which refines itself in areas dense with particles to better resolve the intricate fluid flow around them. We track particle trajectories and link them to specific pores and throats within the rock sample.

Furthermore, we apply a method to compare the pair-wise trajectories of particles with different density, injected in a flux-weighted procedure through the inlet. This allows us to analyze how particle retention varies within the sandstone, considering the flow direction for fines with different densities. For heavier fines, we observe an interesting spatial variation in particle trapping, suggesting that gravity aids their movement in the direction of gravitational pull, but hinders it along the flow path. Our findings reveal that denser fines can move further along the flow path due to two key mechanisms: their ability to pass through gravitationally lower throats and the alterations in flow pathways caused by pore clogging.

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Poster / 505

Evolution characteristics and quantitative model of shale porosity for Wufeng-Longmaxi Formation in southern Sichuan Basin, China

Author: Guangshun Xiao[1]

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Shale is not only a source rock, but also a reservoir rock, and its porosity evolution characteristics have an important influence on the generation, migration and accumulation of oil and gas in the shale formation. By means of integrated experiments of hydrocarbon generation simulation, conventional-overburden porosity analyses, and field emission-scanning electron microscopy (FE-SEM) imaging, the porosity characteristics of Wufeng-Longmaxi Formation at different well locations in southern Sichuan Basin of China were studied. The evolution patterns and influencing factors of inorganic porosity, organic porosity and total porosity were discussed, and a quantitative model of porosity evolution in this area was established. The results show that with the increase of effective pressure, the total porosity gradually decreases, but the rate of decrease gradually slows down, and its variation characteristics are affected by the contents of total organic carbon (TOC) and clay minerals. Inorganic porosity is mainly controlled by burial depth; with the increase of depth, inorganic porosity continuously decreases. In addition, she main factors affecting the extent of organic porosity include TOC contents, organic matter maturity and burial depth. The evolution patterns show that the porosity in this area generally shows a trend of initial rapid decrease, then slow decrease and finally gradual increase. Among them, in the early stage of formation burial, the inorganic porosity decreases rapidly and then slowly, while the organic porosity increases rapidly & slowly and decreases gradually. Furthermore, the overall total porosity decreases continuously, but shows a slow increase trend in the later uplift stage.

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MS11 / 508

Probing into nanoparticles adsorption mechanisms through direct experimental characterization of nanoparticle-pore surface interaction forces

Author: Mingliang Han[None]

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The adsorption of nanoparticles on the pore surface could change surface wettability and slip length, which is dominant for EOR during nanofluid flooding. It is of great value to understand the adsorption mechanism of nanoparticles on the pore surface. The interactions between nanoparticles and pore surface include four significant and common forces, such as Van der Waals force, electrostatic force, attractive hydrophobic force, and repulsive steric force.

Forces were measured directly with the colloidal probe technique of atomic force microscope (AFM), which permits colloidal particles to attach to the cantilever. The forces, obtained in solutions with different salinity, varied from repulsive to attractive, which could be well fitted with the four forces mentioned above. Different forces exert their effects at different distances, among which the action range of Ver der Waals force (about 5 nm) is the least and that of electrostatic force (nearly 40 nm) is the largest. Based on the analysis of the theoretical equations, salinity is the most significant influence factor.

Molecular dynamics simulation was employed to verify the effect of different factors on the interaction between nanoparticle and pore surface. The all-atom models of nanoparticles were modified with alkanes of different densities and lengths to evaluate the repulsive steric force. Different ions with verified concentrations were added to the system to analyze the electrostatic force. The attractive hydrophobic force was assessed by calculating the radial distribution function of water molecules around nanoparticles. The conclusion obtained from molecular dynamics simulation is consistent with the experiment.

The nanoparticles transport with the nanofluids in real pores and throats, meaning the adsorption of nanoparticles is related to the drag force and lift force, which is generated by the flow of liquids. With this fact, the mechanical equilibrium equation of the nanoparticles adsorbed on the surface was established, based on which the maximum adsorption thickness was calculated. The degree of adsorption of the nanoparticle layer on the pore surface could be significantly enhanced by slightly increasing salinity. Our results provide useful insights into the adsorption mechanism of modified nanoparticles on pore surfaces, with important implications for the effective and economical application of nanofluid flooding in different reservoirs.

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MS01 / 509

A Bayesian deep-learning approach to characterize CO2-brine saturation functions from experimental data

Author: Nikolai Andrianov[1]

Co-authors: Behzad Rostami [1]; Samira Mohammadkhani [2]

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An efficient management of a CO2 storage site requires an uncertainty assessment for storage capacity and injectivity. For the case of a saline aquifer onshore Denmark, an unsteady-state core-flooding experiment was conducted in order to assess a potential risk of CO2 injectivity impairment. The experimental results indicate that the rock mineralogy, samples permeability, and samples dimensions were essentially unaffected by CO2 flooding, but precipitated salt and some fines were detected after the end of experiment.

The experimentally obtained differential pressure readings and the brine effluent volume are history-matched to estimate the uncertainty range of the saturation functions for the two-phase water-scCO2 system. The Brooks-Corey (1964) parametrization is used for the relative permeability functions, and the Skjaeveland et al. (1998) parametrization –for the capillary pressure function. The fluid system is modelled with the Peng-Robinson equation of state for the aqueous phase with CO2 dissolution, geochemical reactions, and with salt precipitation. An implementation of this model with a commercial simulator GEM (CMG, 2022) appears to be computationally expensive for multiple forward solutions; a faster simplified two-phase immiscible model, built using MRST (Lie, 2019), is used as a proxy to the full model.

A global search method with multiple starting guesses is used to obtain a number of non-unique solutions to the inverse problem using the MRST model. However, the used forward solver is prohibitively slow for a Bayesian uncertainty quantification of the problem at hand.

A feedforward neural network is set up to approximate the mapping between the tuples of Brooks-Corey-Skjaeveland parameters and the values of the residual between the experimental results and the MRST predictions. The neural network, trained on the convergence history of the global search method, reaches good accuracy overall with Pearson's correlation coefficient up to 0.99 and several orders of magnitude speedup as compared to the forward solver run time.

The history-matched values of the optimization parameters are interpreted as samples of a Gaussian prior distribution. It is shown that the parameters of the capillary function are subject to larger

uncertainty, as compared to the parameters of the relative permeabilities. The posterior distribution is obtained by evaluating the joint distribution for small values of the residual. Using the neural network as a forward problem solver allows to sample the posterior distribution and to obtain the maximum a posteriori estimation of the sought optimization parameters.

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Feature alignment Generative Adversarial Network for Multi-scale fusion reconstruction of Core Images

Author: Pengcheng Yan[None]

Co-authors: Qizhi Teng [1]; Juan Li [1]; Xiaohong Wu [1]; Xiaohai He [1]

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The accurate modeling of the three-dimensional structure of porous media is important for the study of the linkage between the microscopic characteristics and the macroscopic physical properties/phenomena. Multi-scale pore structures are widely distributed in nature and industry. However, due to the tradeoff between field of view (FOV) and resolution, it is difficult to obtain high-resolution images with a large field of view in a single imaging process. High-resolution images with small field of view can capture more detailed features, but lack representation of the entire microstructure. Low-resolution structures with a large field of view are more representative, but lack detailed features. Multi-scale fusion reconstruction is an effective way to model large-view and high-resolution structures. Previous studies have shown that the method based on deep learning in particular has great potential in multi-scale reconstruction. In this paper, we propose a feature alignment Generative Adversarial Network (FAGAN) to achieve multi-scale fusion modeling of digital core images, which combines 2D small-FOV high-resolution images (2D HRI) and 3D large-FOV low-resolution images (3D LRI). There are dimensional differences between 2D image features and 3D image features, and 3D feature space can represent 3D spatial structure more accurately. Therefore, the generator of FA-GAN uses a two-stream network to extract the semantic features of 3D LRI and 2D HRI respectively. A feature reconstruction module is designed to convert 2D image feature F_{2D} into 3D feature representation $F_{(2D\sim3D)}$, so as to realize the feature fusion of 2D HRI and 3D LRI in 3D feature space. The semantic consistency of F_{2D} and $F_{(2D\sim3D)}$ is constrained by combining the feature space alignment loss function (FSAloss). In addition, a feature alignment module is designed to align $F_{(2D\sim3D)}$ with 3D LRI semantic feature F_{3D} to ensure the correct fusion of features. The visualization results show that the structure generated by the model follows both the spatial geometry of 3D LRI and the fine details of 2D HRI. The validity of the reconstructed results is further verified by the statistical parameters (two-point correlation function, pore diameter distribution, shape factor distribution, etc.) and numerical analysis (permeability, etc.) of the reconstruction structure and the real structure.

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Organic matter–oil adhesion force and ultimate flow distance of adsorbed oil in shale reservoirs

Author: Rui Shen[1]

Co-authors: Lei Xu [2]; Hang Yang [1]; Shengchun Xiong [1]

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In China, continental shale oil reservoirs are featured with extremely low porosity and permeability, where oil is greatly subjected to solid–liquid adhesion force. The organic matter–oil adhesion force plays a crucial role in shale oil occurrence and movability in shale reservoirs. To effectively characterize the organic matter–oil adhesion force, this paper presents an AFM testing method to measure the adhesion force and derives the formula of pressure distribution with the adhesion force as the major flow resistance. It is found that organic matter shows the largest roughness, followed by felsic; and pyrites and interstitial materials show the smallest roughness. Organic matter exhibits larger average grain size, but smaller pore number than felsic. Given a similar organic matter maturity, the organic matter–oil adhesion force decreases with increasing content of light components. If pore wall length in organic matter is larger than the ultimate flow distance, adsorbed oil will not be desorbed to form free oil; on the contrary, adsorbed oil will be desorbed and turn into free oil. Hydraulic fracturing can raise reservoir pressure and the ultimate flow distance of adsorbed oil, thus allowing more adsorbed oil to be produced.

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Mechanism of EOR and evaluation of carbon capture by alternating injection of methane-enriched associated gas and CO2 on a deep oil reservoir

Authors: Yifan ma[1]; Zongfa Li[1]; HUi Zhao[1]; Lijuan Huang[1]; Zifeng Chen[1]

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The feasibility of CO2-assisted associated gas in enhancing oil recovery is discussed. Firstly, one-dimensional gas flooding experiments are performed under 50 MPa and 112 ℃. Results show that CO2 flooding, natural gas flooding, associated gas flooding, and N2 flooding can recover 90.3%, 88.3%, 75.5%, and 60.7% oil, respectively. Secondly, numerical simulations of gas flooding at field scale are conducted. Analysis show that enhanced cumulative oil production of gas flooding is determined by oil components extraction effect and gas flooding swept area. The oil components extraction effect of CO2 is better than natural gas, but CO2 flooding swept area is the smallest among CO2 flooding, natural gas flooding, associated gas flooding, and N2 flooding. The swept area of associated gas flooding and N2 flooding is larger than natural gas, but their oil components extraction effects are too low. Therefore, the enhanced cumulative oil production of natural gas flooding is the highest. Finally, gas components optimization is conducted using particle swarm optimization, genetic algorithm, simulated annealing algorithm, and surrogate optimization. Optimization results show that gas composed of about 20 mol.% CO2 and 80 mol.% associated gas can coordinate oil components extraction and swept area best. The cumulative oil production of optimized gas flooding is about 6.4%, 2.0%, and 0.3% higher than associated gas flooding, CO2 flooding, and natural gas flooding, respectively. The study provides valuable guidance for enhancing cumulative oil production, sequestrating CO2, and recycling associated gas.

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Differences in acid dissolution patterns of carbonate reservoirs with different dimensions

Author: Xuhang Su[1]

Co-authors: Ning Qi [1]; Xiangke Shi [2]; Yixin Lu [1]; Xuesong Li [1]

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Acidizing and acid fracturing are important production enhancement measures for reservoir stimulation in carbonate reservoirs, and the numerical simulation method is often used to study the mechanism of acid dissolution. In the numerical simulation of acid dissolution in carbonate reservoirs, the three-dimensional model can better reflect the details of acid-etched morphology than the two-dimensional model. Furthermore, the three-dimensional model considers the heterogeneity in the third direction, so it can obtain a more realistic acid-etched morphology, which is conducive to achieving a precise simulation of acid dissolution. However, compared with the two-dimensional model, the large number of grids in the three-dimensional model leads to problems such as high computational workload, low computational efficiency, and poor convergence of results. To clarify the accuracy difference between the two-dimensional and three-dimensional models, the distribution diagrams of the two-dimensional model under the same conditions are compared with the cross-sectional distribution diagrams of the three-dimensional model, and the specific reasons for the accuracy difference are identified. In addition, there are differences in breakthrough volumes between the two-dimensional and three-dimensional models under different dissolution patterns. When they are face, conical, ramified, and uniform dissolutions, the breakthrough volumes of the two models are similar. However, when it is wormhole dissolution, the breakthrough volumes of the two models differ significantly.

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MS06-B / 519

Evaporation in porous media with salt precipitation

Author: Rui Wu[1]

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Visualization experiments are performed to disclose the salt precipitation and gas-liquid displacement in microfluidic pore networks during evaporation. Two forms of salt precipitation are revealed: aggregated polycrystalline structures and large bulk crystals. It is found that gas bubbles can be formed because of imbibition of liquid into aggregated polycrystalline structures. The length of a corner liquid film can affect the direction of growth of the aggregated polycrystalline structures connected to the corner liquid film. Discontinuous corner liquid films can be transformed to continuous ones when they are touched by growing aggregated polycrystalline structures. The “sleeping” aggregated polycrystalline structures at the open surface of a microfluidic pore network, i.e. efflorescence, can grow again if they are touched by growing aggregated polycrystalline structures inside the microfluidic pore network, i.e. subflorescence. Because of efflorescence, the evaporation rate from a microfluidic pore network can increase first and then decrease. In addtion, the distribution of the precipitated salts also depends on the thermal gradient along the microfluid pore networks.

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Poster / 523

Study on Reservoir Time-Varying Patterns and Remaining Oil Distribution in Sandstone Reservoirs during Long-Term Water Flooding Process

Author: Tonghui Liu[1]

Co-author: Yongfei Yang [1]

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The medium-high permeability sandstone reservoir has the advantages of high permeability and porosity, low cementation degree, and strong oil and gas migration ability. The reservoir rocks are mainly composed of clay minerals and fine silty particles. In the long-term water flooding development process, the scouring effect of water will cause clay minerals to fall off and migrate, and the reservoir structure and properties will change, thus altering the oil displacement mechanism.
To improve the understanding of the change in rock physical properties and the capture and migration mechanism of internal multiphase flow during long-term water flooding, experiments on sandstone cores with different permeability and porosity were carried out. Based on CT scanning technology, the pore network model is constructed to study the change in rock pore throat structure during high-speed and long-term water flooding. Combined with X-ray diffraction, SEM images, and core flow experiments, the evolution mechanism of reservoir physical properties is discussed. On this basis, the occurrence types, distribution characteristics, and formation mechanism of microscopic remaining oil are studied, and the distribution characteristics of remaining oil in long-term

water flooding and short-term water flooding are compared.
The results indicate that the heterogeneity of the core pore structure affects the location and morphology of residual oil, resulting in different dominant types of residual oil within sandstone cores with varying permeability. In addition, the improvement of pore throat structure and the transformation of wettability are inherent reasons for long-term water flooding to improve oil recovery efficiency.

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MS03 / **524**

A pore-scale investigation of dispersion in two-phase flow with varied viscosity contrast in porous media

Author: Zijing LI[1]

Co-authors: TETSUYA SUEKANE ; Chunwei Zhang [2]

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Dispersion in partially saturated porous media has many applications in scientific and engineering fields. For example, in carbon dioxide capture and storage (CCS), dispersion increases the mass transfer rate and accelerates the dissolution process in large background velocity field (Tsinober, 2022). In this study, we create a steady-state system that mimics a depleted oil field where salty water and oil co-exist. A tracer cloud is injected into a cylindrical container where sands are densely packed, representing a supercritical CO2 cloud that can mix with the surrounding water in a porous media. The impact of oil viscosity on dispersion behaviors was investigated in a large range of viscosity contrast of non-wetting phase and wetting phase from 0.65 to 500.
The results inform dispersion scale was drastically extended with the increase of viscosity contrast. An increase in viscosity contrast yields more heterogeneities of the local velocity field generated by trapped oil with a wide variation of its volumes. The local heterogeneity causes surface distortions and increases the interfacial area of the tracer cloud and surrounding brine water. The dispersion coefficients vary with time and exhibit abnormal behaviors, especially when the oil viscosity is large. These results can be attributed to the fact that the oil phase becomes disconnected, and the volume of trapped oil decreases as the oil viscosity increases (Suwandi et al., 2022). An oil film is observed, where oil is sandwiched by sand and water and narrows pore spaces. The velocity of the water phase exhibits an extensive range of fluctuation, which may contribute to the enhanced dispersion and mixing state, even with the low connectivity of the water phase.
This study provides insights into dispersion in porous media where oil and water co-exist with varied oil viscosities at both the large and pore scales, which may provide an insight into the storage condition of CO2 in partially saturated porous media (Li, 2022).

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References:

Li, Y. et al. (2022). In-Situ Imaging of CO2 Trapping and Oil Recovery in Three-Phase Systems: Dependence on Pore Geometry and Wettability. SPE Journal, 1–15. Suwandi, N., Jiang, F., & Tsuji, T. (2022). Relative Permeability Variation Depending on Viscosity Ratio and Capillary Number. Water Resources Research, 58(6). https://doi.org/10.1029/2021WR031501 Tsinober, Avihai, Ravid Rosenzweig, Holger Class, Rainer Helmig, and U. S. (2022). The Role of Mixed Convection and Hydrodynamic Dispersion During CO2 Dissolution in Saline Aquifers: A Numerical Study. Water Resources Research, 58(3), e2021WR030494. https://doi.org/10.1029/2021WR030494

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Poster / 525

Modelling liquid-gas interface movement under imbibition conditions considering solubility effects

Authors: Xingfu Li[1]; Shitao Liu[1]; Igor Shikhov[1]; Christoph Arns[1]

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The geological storage of CO2 involves the interaction of non-equilibrated fluids (connate water and injected fluid) which then equilibrate over time. The CO2 phase diagram and solubility of CO2 in water adds significant complexity to this process. Namely, the existence of concentration gradients surrounding fluid-fluid interfaces may impact on wettability or more general on surface conditions. These pore-scale mechanisms make the prediction of fluid movements a challenging task.
Our research investigates the behaviour of the gas-liquid interface due to the variation in solubility dynamics by numerically simulating the spontaneous capillary imbibition of water into a gas-filled medium. An open-source simulation software featuring the "hybridPorousInterFoam" package is utilized, where the formation of two-phase interfaces is achieved by setting the initial fluid distribution and using the VOF (Volume of Fluid) method to calculate the liquid volume fraction in each cell, thereby accurately tracking the fluid-gas interface positions between as well as calculating the changing fractional fluid composition on either side of the moving interface. Subsequently, the simulation accurately reflects the physical behaviour at these interfaces by incorporating the effects of capillary forces and gravity.
This package allows the input of a distribution of contact angles to set the boundary conditions on the solid surface. Here we introduce additional functionality to model the concentration gradient evolution around the moving interfaces and account for the change in contact angles accordingly.
We demonstrate the capabilities of the new solver packages on a set of basic geometries, investigating the impact of solubility (e.g., due to temperature variations) on the resultant fluid configurations and displacement efficiency.

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Carrillo, F. J., Bourg, I. C., & Soulaine, C. (2020). Multiphase flow modeling in multiscale porous media: An open-source micro-continuum approach. Journal of Computational Physics: X, 8, 100073.

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MS17 / **526**

A pore-scale perspective on the hydraulic fracturing of heterogeneous glutenites

Authors: yanying chen[1]; Hongqing Song[2]; Chiyu Xie[2]

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[2] *School of Civil and Resource Engineering, University of Science and Technology Beiing*

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Hydraulic fracturing is one of the most important technique for the development of tight glutenite reservoirs. The strong heterogeneity of the sand and gravel particles make it difficult to comprehensively understand the fracturing mechanisms of glutenites. Most of the existing studies have been mainly focused on the effects of injection rate1, stress differential2, and fracturing fluid viscosity[3], However, there still lacks a systematic consideration of the impact of glutenite heterogeneity especially on the aspects of matrix and gravel bonding interface strength and gravel mechanical properties.

Therefore, the aim of this study is to reveal the effects of interface bonding strength and gravel properties on the fracture evolution of glutenite at the pore scale. The heterogeneity of the matrix, gravel particle, and interface strength are considered by a global cohesive zone model. Heterogeneity is achieved by assigning different strengths and critical fracture energies to the cohesive elements of matrix, gravel, and interface. The simulation is validated by comparing the results with existing experimental observations[4].

We first discussed the fracturing of a model glutenite with the same size gravel particles but different interface bonding strength and gravel properties. We established a phase diagram to fast evaluate the crack propagation mode by using the ratios of critical tensile energy of gravel to matrix and matrix to surface. To get closer to the real glutenites, we also considered more complexed glutenites composed of three kinds of gravels with different sizes, bonding strengths and mechanical properties. Modeling results indicate that hydraulic fractures tend to propagate along the path with the minimum critical fracture energy. The differences in strength between gravel and interface lead to alterations in the propagation path and speed of hydraulic fractures, significantly impacting the length of hydraulic fractures.

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1Sharafisafa Mansour,Aliabadian Zeinab,Sato Akira Shen Luming.(2023).Coupled Thermo-hydro-mechanical Simulation of Hydraulic Fracturing in Deep Reservoirs Using Finite-Discrete Element Method.Rock Mechanics and Rock Engineering(7),5039-5075. 2Weiwei Zhu,Zhiqiang Chen,Xupeng He,Zhiguo Tian Moran Wang.(2023).Numerical Investigation of Influential Factors in Hydraulic Fracturing Processes Using Coupled Discrete Element-Lattice Boltzmann Method.Journal of Geophysical Research: Solid Earth(9). [3]Xian S ,Yong Q ,Hongxing X , et al.Numerical simulation of hydraulic fracture propagation in conglomerate reservoirs[J].Engineering Fracture Mechanics,2021,248 [4]Xinfang Ma,Yushi Zou,Ning Li,Ming Chen,Yinuo Zhang Zizhong Liu.(2017).Experimental study on the mechanism of hydraulic fracture growth in a glutenite reservoir.Journal of Structural Geology37-47

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Poster / **527**

Application of 2D and 3D imaging technology in the observation of porous media containing natural gas hydrates

Authors: Chengfeng Li[None]; Jianye Sun[1]; Xiluo Hao[1]; Yongchao Zhang[1]; Lele Liu[1]

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Natural gas hydrate is a potential new type of energy, mainly found in sediments in marine or terrestrial permafrost regions. The content, distribution, and growth or decomposition of natural gas hydrates in sediment pores or fractures, greatly affect the physical properties of the medium. This study mainly introduces the experimental techniques and methods for micro and nano scale imaging of porous media containing natural gas hydrates based on Micro-CT and Cryo-SEM. In response to the observation needs of natural gas hydrates at low temperature or high pressure, a dedicated auxiliary observation container has been independently developed, which can observe the microscopic morphological changes of hydrate growth and decomposition processes. At the same time, a non-destructive transfer device suitable for CT and SEM scanning was also designed, aimed at conducting CT and SEM imaging observations on the same sample, achieving joint observation of CT images and SEM images. In addition, a fusion method for micrometer and nanoscale digital core images has been developed, which utilizes self supervised learning algorithms in machine learning to achieve a 2x and 4x increase in spatial resolution of CT images.

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MS01 / **528**

Numerical simulation of depleted and cushion gases impacts on hydrogen storage in a depleted gas reservoir

Authors: Yawen Yang[1]; Hua Tian[2]; Yongfei Yang[3]; Kai Liu[1]; WeiYao Zhu[1]; Stefan Iglauer[4]; Bin Pan[1]

[1] *University of Science and Technology Beijing*

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

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

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Depleted gas reservoirs have large storage capacity, pre-proved containment security, in-place depleted gas, and well-established surface infrastructures, thus are viewed as the most feasible hydrogen storage space. However, the impacts of depletion time, volume ratio ($VR_{H_2:CH_4/CO_2}$) of hydrogen (H_2), depleted gas (mainly CH_4) and cushion gas (e.g., CO_2), and injection/withdrawal mode on hydrogen storage performance have not been systematically studied. Therefore, we examined these impacts using a numerical simulation method. The results demonstrate that: 1) As the $VR_{H_2:CH_4}$ decreases from 100% : 0 to 50% : 50%, both H_2 withdrawal factor (W_{F-H_2}) and purity (W_{P-H_2}) firstly increase and then decrease; during the 1^{st} withdrawal cycle, the highest W_{F-H_2} is 42% and the smallest W_{P-H_2} is 51%, both of which occur at the $VR_{H_2:CH_4}$ = 60% : 40%. 2) In case of CO_2 as cushion gas, W_{F-H_2} and W_{P-H_2} are decrease as the $VR_{H_2:CO_2}$ increases from 50% : 50% to 25% : 75%; during the 1^{st} withdrawal cycle, the highest W_{F-H_2} is 38% and the smallest W_{P-H_2} is 50%, both of which occur at the $VR_{H_2:CO_2}$ = 25% : 75%. 3) A smaller H_2 withdrawal rate (W_{R-H_2}) results in a lower W_{F-H_2}, but a higher W_{P-H_2}, e.g., at the $VR_{H_2:CH_4}$ = 60% : 40%, W_{F-H_2} and W_{P-H_2} are 42% and 51% at W_{R-H_2} = 100×10^4 Sm^3/day, respectively, while they become 31% and 64%, respectively, at W_{R-H_2} = 50×10^4 Sm^3/day. These simulation results indicate that cushion gas injection is beneficial to reducing hydrogen loss, and depleted gas can be used as cushion gas. Depletion time and the ratio of hydrogen, depleted and cushion gas have significant influence on hydrogen storage performance. These insights provide important guidance for industrial hydrogen storage in depleted gas reservoirs.

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MS07 / **532**

Thermodynamically consistent modeling and simulation of two-phase flow and multicomponent flow in porous media with rock compressibility

Author: Huangxin Chen[1]

[1] *Xiamen University*

Corresponding Author: chx@xmu.edu.cn

In this talk we will introduce a thermodynamically consistent mathematical model for incompressible and immiscible two-phase flow in porous media with rock compressibility. An energy stable numerical method will be introduced, which can preserve multiple physical properties, including the energy dissipation law, full conservation law for both fluids and pore volumes, and bounds of porosity and saturations. Furthermore, an energy-stable and conservative numerical method for multicomponent Maxwell-Stefan model with rock compressibility will also be discussed.

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MS09 / **536**

Lattice Boltzmann modeling of pore-scale fluid flow during wettability alteration-based enhanced oil recovery in marine porous carbonate reservoirs

Authors: Daigang Wang[None]; Fangzhou Liu[None]; Yong Li[None]; Zhe Hu[None]; Kaoping Song[None]

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The Middle East has become the largest overseas oil production base of China, where marine porous carbonate reservoirs are widely-distributed. Large recoverable reserves are still unexploited, implying a great potential to obtain higher oil production. Influenced by pore type, multi-modal pore structure, initially oil-wet or mixed-wet condition, the microscopic displacement efficiency is relatively low, only 40%~60%. Using ion-matched surfactant flooding to carry out wettability control from initially oil-wet or mixed-wet to water-wet, oil recovery ratio of marine carbonate reservoirs can be remarkably increased. Ion-matched surfactant flooding has been regarded as an attractive technique to greatly improve oil recovery after waterflooding in marine carbonate reservoirs. However, pore-scale mathematical models of wettability control by ion-matched surfactant flooding have not been reported in the literature. It is unclear about the pore-scale fluid flow mechanism during wettability control.

To tackle these issues, core samples from a typical carbonate reservoir in the Middle East were selected. Multi-modal pore structure image data were acquired by micro-focus X-ray CT scans. The study employed the U-Net fully convolutional neural network deep learning semantic segmentation algorithm. With a limited amount of image data, it accurately identified and constructed a digitized core model of the multi-modal pore structure. A pore-scale fluid flow mathematical model for LSW-S system infiltration control and lattice Boltzmann simulation method were then established by describing major physical-chemical processes such as oil/water two-phase flow, wettability alteration, solute convection-diffusion, surfactant adsorption/desorption and reducing oil/water interfacial tension. By comparing with classical equation analytical solutions, the accuracy of the simulation results was verified. The study investigated the impact of factors on pore-scale fluid flow characteristics of enhanced oil recovery through infiltration control, including displacement system, ion-concentration, capillary number, and wettability .
The research results indicated that due to local adsorption-desorption imbalance, both LSW drive and LSW-S drive caused dynamic changes in rock wettability, effectively detaching oil film but without altering the flow path of the displacing medium. In porous carbonate rocks, the sequence of pore-scale oil displacement efficiency was: LSW-S > LSW > HSW. A lower concentration of ion-matched water facilitated the detachment of oil films and droplets from small pores. A lower concentration of ion-matched water was more conducive to detaching oil films and droplets from small pores. Ion concentration mainly affected the relative permeability of the oil phase and had a minor impact on the relative permeability of the water phase. The capillary number had a significant impact on oil displacement efficiency and fluid microscopic distribution. As the capillary number increased, the force of fluid driving increased, leading to a significant increase in both oil and water relative permeabilities. With rock wettability transitioning from oil-wet to neutral wetting, the oil phase's relative permeability increased, while the water phase's relative permeability decreased. Under neutral wetting conditions, ion-matched water exhibited pronounced effects on infiltration control, substantially increasing the relative permeability of the oil phase and mobilizing microscopic residual oil.

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Poster / **537**

Oscillation Method for Measuring Gas Storage in MCM-41

Authors: Muhammad Airlangga[1]; John Sass[2]; Nolan Kovach[2]; Brian Trewyn[2]; Xiaolong Yin[3]

[1] *Pertamina Hulu Energy*

[2] *Colorado School of Mines*

[3] *Eastern Institute of Technology, Ningbo*

Corresponding Author: xyin@eitech.edu.cn

The total storage of gas in a mesoporous material MCM-41 with adsorption/capillary condensation was measured using a new oscillation-based method. With an improved setup and procedure, the accuracy of the measured isotherm was significantly improved. Experiments were conducted using both condensable (propane and carbon dioxide) and non-condensable (argon and methane) gases. The results show that this method can be used to measure not only the total storage of gas but also the excess due to adsorption/capillary condensation with considerable accuracy. In experiments conducted with propane, the occurrence of capillary condensation, which increased the total storage of gas, was well depicted.

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Poster / 539

Wave Velocity Dispersion and Attenuation in Partially Saturated Porous Media

Author: Jimmy Xuekai Li[1]

Co-authors: Jinghao Hu [1]; Seyederfan Saberhosseini [1]; Tiancheng Zhang [1]; Zhongwei Chen [1]

[1] *The University of Queensland*

Corresponding Authors: zhongwei.chen@uq.edu.au, jinghao.hu@uq.edu.au, s.saberhosseini@uq.edu.au, tiancheng.zhang@uq.edu.a

The understanding of the seismic signature of the partially saturated formation is critical to seismic monitoring in the hydrogen geo-storage, CO2 geo-sequestration and geophysical survey and exploration of oil and gas reservoir. The main objective of this study is to model the wave propagation in partially saturated rocks containing two immiscible fluids (i.e., gas-water), with a comparative case study on hydrogen (H2), methane (CH4), nitrogen (N2) and carbon dioxide (CO2) bearing rocks. The sonic velocities and the attenuations are influenced by several parameters, which interact in a complex pattern, particularly when the rock is saturated with multiple fluids. We developed a rock physics model that considers the effects of patchy saturation, wettability, effective pressure, and relative permeability. By examining wave propagation in each fluid-saturated case against water saturation, we improve our understanding of changes in sonic velocity and attenuation during the water saturation varies. This provides valuable insights for seismic and sonic monitoring during the injection and extraction of gas in the reservoir formation.

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MS10 / **540**

Quantifying the effective porosity of reservoir and source rocks: Multi-scale and multi-approach studies

Authors: Qinhong Hu[1]; Qiming Wang[None]; Tao Zhang[None]; Shengyu Yang[None]; Chen Zhao[None]

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

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Microscopic pore structure characteristics of both reservoir and source rocks (e.g., sandstones, carbonates, and mudrocks) –pore-size distribution, pore shape, and pore connectivity –control fluid flow and chemical transport. Focusing on effective porosity, the portion of connected pore space as conductive pathways to participate in flow and transport (e „ as an indicator of macroscopic connectivity), this presentation discusses various approaches to quantifying the effective porosity for a range of oil and gas reservoir and source rocks. The approaches include pycnometry (liquid and gas), pore and bulk volume measurement after vacuum saturation, porosimetry (mercury intrusion porosimetry, low-pressure gas physisorption isotherm, water vapor adsorption/desorption isotherm, nuclear magnetic resonance cyroporometry), imaging (X-ray computed tomography, Wood's metal impregnation, field emission-scanning electron microscopy SEM, focus ion beam-SEM), scattering (ultra- and small-angle neutron and X-ray), 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. Our results indicate a disparate characteristics and range of effective porosity, with a single-zone behavior and a value of connectivity at approximately 70% for sandstones, as compared to "dual-connectivity zones" at 70% and 0.01% for organic matter-rich mudrocks.

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MS01 / 541

Effect of dissolution and heterogeneity on supercritical CO2 invasion in porous media: an experimental study using X-ray micro-computed tomographic imaging

Author: Ruotong Huang[None]

Co-authors: Anna Herring [1]; Adrian Sheppard [2]; Mohammad Saadatfar [3]

[1] *University of Tennessee*

[2] *Australian National University*

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In this study, with the utilization of quasi-dynamic X-ray micro-computed tomographic (MCT) imaging, pore-scale fluid configurations were tracked for CO_2 injected into two different brine-saturated Bentheimer sandstone cores under conditions relevant to geologic carbon sequestration. CO_2 injection was performed at low capillary number (Ca = 10^{-9}) into cores saturated with live- and dead-brine, consecutively. Two cores with different pore space characteristics were used to investigate the impact of heterogeneity on the resultant fluid configurations. We also interrogated possible wettability alteration during CO_2 injection based on the obtained MCT images. We find that invasion patterns continue to evolve long after breakthrough, with distinct and gradual saturation changes occurring after decades of pore volumes injected. For one core, the invasion patterns for both live- and dead-brine conditions eventually converge after 16.5 pore volumes; for the second core, the patterns are distinct under the different injection conditions for up to 30.1 pore volumes. The presence of pore-scale heterogeneities in the cores has a strong influence on the ultimate CO_2 distribution under the different conditions. It is expected that results from this study will contribute to better understanding of the pore-scale invasion of CO_2 and ultimately, the field-scale application of geologic carbon sequestration.

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542

Parallel thermo-hydro-mechanical coupling simulations based on an embedded discrete fracture model on unstructured grids.

Authors: Tong Wang[1]; Jun Yao[1]

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

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In this work, a parallel thermo-hydro-mechanic coupling reservoir simulation approach is developed using an embedded discrete fracture model (EDFM) on unstructured grids. For the thermo-hydro-mechanical coupling problem, the finite volume method is adopted to discretize compositional flow, heat transform and poro-mechanical equations uniformly. In addition, a sequential implicit method is employed to solve the nonlinear coupling problem. Moreover, the proposed simulation method is massively parallelized based on a domain decomposition approach. A load-balanced domain decomposition algorithm is proposed to improve the parallel efficiency, this algorithm can eliminate the unbalance caused by the nonuniform distribution of fractures and the difference of the sparsity of fracture discretization stencil. A tiling technique and a non-blocking communication approach are implemented for the block sparse matrix-vector multiplication operator used in linear solving. Finally, this simulator is used for high-resolution parallel simulations in different engineering scenarios, including a multi-layer shale gas reservoir three-dimensional simulation and a deep high-temperature fractured reservoir simulation. The parallel computational performance and scalability are analyzed at different parallel scales.

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MS21 / 543

Incorporating Pore Size Distribution into Dynamic Permeability Modelling for Porous Media

Author: Jimmy Xuekai Li[1]

Co-authors: Mohammad Sarmadivaleh [2]; Reza Rezaee [2]; Tobias M. Müller [3]

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Previous dynamic permeability models often relied on simplified and assumed pore-scale parameters such as average pore radius, potentially leading to inaccuracies. This study introduces a novel approach that directly incorporates measured pore size distributions, addressing these limitations and providing a more realistic representation of fluid flow in porous media. Key findings include:

- Pore size distribution's primary impact on dynamic permeability: The model demonstrates that pore size and its distribution exert a first-order effect on dynamic permeability.
- Integration of measurable pore size data: The model utilizes pore size distributions obtained from techniques like MICP or NMR, enabling direct incorporation of measured data for enhanced model accuracy and applicability.
- Incorporation of slip boundary conditions for wettability effects: The model accounts for wettability's influence on dynamic permeability, providing a more comprehensive understanding of fluid flow behaviour in porous media with varying wettability characteristics.

Overall, this study presents a practical dynamic permeability model that overcomes limitations of existing approaches by incorporating pore size distribution and wettability effects. This model holds significant potential for improved characterization and understanding of fluid flow in diverse porous media applications, potentially leading to advancements in various fields.

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MS20 / **547**

Cardiac Microvascular Obstruction: microvascular drug transport and lysis of microthrombi in a multi-scale model of the myocardial microcirculation

Author: Yannick Rösch[1]

Co-authors: Anastasia Milusev [1]; Petra Wolint [2]; Miriam Weisskopf [3]; Nikola Cesarovic [2]; Dominik Obrist [1]

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Cardiac microvascular obstruction (MVO) is an injury of the myocardial microcirculation. It typically follows successful recanalization of the blocked coronary artery (primary occlusion) in myocardial infarction. MVO leads to under-perfusion of the affected tissue and has a negative impact on patient outcomes. Next to other occluding factors, MVO may be caused by microthrombi (debris from the primary occlusion) embolizing vessels of less than 200µm diameter 1.
For the systematic study of MVO and to test diagnostic and therapeutic approaches, we have developed a multi-scale in vitro model for MVO 2. It comprises a microfluidic chip modeling a branching

microvascular tree with vessel diameters ranging from 700 to 50µm. The chip is integrated into a model of the coronary circulation which is coupled to a left-heart mock loop. This experimental setup provides physiological flow conditions for the whole model. MVO is induced by injecting porcine microthrombi (~200µm) into the microfluidic chip where they randomly distribute and embolize some of the microchannels [3].
Infusion experiments with dye indicated that some microthrombi lead to a full occlusion of the respective microchannel such that mass transport toward the occluding microthrombus is very inefficient, whereas other microthrombi have a semi-occlusive or porous character such that advective transport toward the microthrombus is possible. Furthermore, we found that periodic fluctuations of the vessel volume, due to the contraction of the myocardium with every heartbeat, enable mass transport also in occluded vessels (intramyocardial pumping effect, [4]), like squeezing and soaking a dishwashing sponge.
Results from the dye infusion experiments suggest that it is possible to transport thrombolytic drugs to the microthrombi such that they can resolve the occlusions and help to reestablish blood perfusion to the myocardium. To identify the appropriate drug infusion protocol and the optimal drug dosages, we developed a second microfluidic setup with a single straight microchannel and constant flow. It ensures that the microthrombi in the chip are non-occlusive such that the drug can always reach the microthrombi. We found that microthrombi can be lysed up to 75% over the course of 20 minutes of perfusion if the thrombi are first exposed to a high drug concentration (alteplase) for 90 seconds. These results will be applied to the experimental setup with the full microvascular tree and intramyocardial pumping effect.

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MS17 / 549

Clathrate Hydrates in Porous Media: Application to Low-carbon Fuels in Clean Energy Transition

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Carbon capture and sequestration (CCS) plays a crucial role in facilitating low-carbon fuel adoption during the clean energy transition. Clathrate hydrates are solid compounds consisting of gas molecules enclathrated in crystalline lattices formed by water molecules. Specifically, CO2 hydrate has become an attractive way for CO2 capture, storage and long-term sequestration. For CO2 capture, fixed bed reactor (FBR) configuration using porous media was reported to significantly enhance the kinetics of the hydrate-based CO2 separation process. Porous media are beneficial as they can provide more hydrate nucleation sites, tortuous pathways for fluid diffusion and sufficient gas-water contact area. On the other hand, forming CO2 hydrates in deep marine sediment offers a secure solution for long-term carbon sequestration due to their higher density than seawater, high stability under moderate oceanic depths, and low susceptibility to oceanic flow perturbation. It is also possible to sequestrate CO2 in natural gas hydrate reservoirs via CO2-CH4 swapping and bring more economic benefits by recovering natural gas. This work will highlight the research efforts carried out by our group in the aforementioned aspects [1-6] and discuss the key roles of porous media in these hydrate processes. The major challenges and prospects are also identified and highlighted.

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1 Zheng J, Lee YK, Babu P, Zhang P, Linga P. Impact of fixed bed reactor orientation, liquid saturation, bed volume and temperature on the clathrate hydrate process for pre-combustion carbon capture. Journal of Natural Gas Science and Engineering. 2016;35:1499-510. 2 Zheng J, Zhang B-Y, Wu Q, Linga P. Kinetic Evaluation of Cyclopentane as a Promoter for CO2 Capture via a Clathrate Process Employing Different Contact Modes. ACS Sustainable Chemistry & Engineering. 2018;6(9):11913-21. [3] Fahed Qureshi M, Zheng J, Khandelwal H, Venkataraman P, Usadi A, Barckholtz TA, et al. Laboratory demonstration of the stability of CO2 hydrates in deep-oceanic sediments. Chemical Engineering Journal. 2022;432:134290. [4] Zheng J, Chong ZR, Qureshi MF, Linga P. Carbon Dioxide Sequestration via Gas Hydrates: A Potential Pathway toward Decarbonization. Energy & Fuels. 2020;34(9):10529-46. [5] Liao Y, Zheng J, Wang Z, Sun B, Sun X, Linga P. Modeling and characterizing the thermal and kinetic behavior of methane hydrate dissociation in sandy porous media. Applied Energy. 2022;312:118804. [6] Liu Z, Zheng J, Wang Z, Gao Y, Sun B, Liao Y, et al. Effect of clay on methane hydrate formation and dissociation in sediment: Implications for energy recovery from clayey-sandy hydrate reservoirs. Applied Energy. 2023;341:121064.

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551

In situ determination of diffusion coefficients of CO2, SF6 gas mixtures in brine

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Tracer monitoring technology is an effective means to detect and quantify the transport and leakage in the CO2 storage process, which has been applied in the traditional oil and gas industry to achieve certain results, but has not yet been successfully applied on a large scale in subsea storage. Diffusion coefficient is an important parameter for analyzing the diffusion performance of CO2 tracer system, so there is an urgent need to establish the test technology of CO2 and tracer transport in reservoir to obtain the diffusion coefficients of CO2 and tracer. It is also necessary to analyze the influence of different tracer concentrations on the diffusion performance of tracer to determine the most suitable tracer concentration.SF6 is chemically stable, has a low environmental background value, and has a low adsorption amount in saline water layer; it has the same symmetric structure and closer molecular weight than CO2, similar physical properties, and good tracer compatibility; and it can be analyzed by infrared detector on-line, so SF6 is chosen as the tracer of CO2 in this study. Therefore, SF6 was chosen as the tracer of CO2 in this study. In this study, diffusion experiments were carried out in transparent high-pressure quartz capillaries at different temperatures and pressures with different gas mixture ratios in brine solutions of different concentrations, and the micro-laser Raman spectroscopy in-situ testing technique was used to monitor the change of gas concentration in the solution over time during the diffusion process in real time, calculate the diffusion coefficients under the conditions of oceanic sequestration, and analyze the effects of various factors on the diffusion coefficients. A model was also established to describe the relationship between the diffusion coefficient and the concentration of tracer added to determine the most suitable concentration of tracer added.

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552

Experimental Study on the Mechanism of Enhanced Oil Recovery by Imbibition Synergism in Tight Oil Displacement

Authors: Yanan Zhang[1]; Yuliang Su[None]; Guanglin Yu[None]; Wendong Wang[None]

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Due to extremely low permeability and undeveloped porosity in tight oil/gas reservoirs, hydraulic fracturing is commonly used for efficient development. Displacement under pressure difference and imbibition under capillary forces continuously occur in the matrix and fractures, facilitating oil displacement by water. We employed CT online scanning and nuclear magnetic resonance for experimental setups, studying pressurized imbibition in fracture/matrix and integrated displacement-imbibition. These setups were instrumental in calibrating the ranges of action during tight oil displacement and imbibition processes, providing insights into energy storage mechanisms and factors influencing enhanced oil recovery from hydraulic fracturing.

Through CT online scanning pressurized imbibition experiments and integrated displacement-imbibition experiments on fracture/matrix cores, we investigated imbibition mechanisms and the impact of hydraulic fracturing on enhanced oil recovery. Real-time observation in CT experiments clarified imbibition distances for matrix and fracture cores, revealing varied recovery rates. A multi-core device was designed to simulate the displacement-imbibition process in reservoirs with paths such as injection well-production well and fracture zone-matrix tight zone. Nuclear magnetic resonance was utilized to monitor the degree of utilization of different pore throats before and after displacement-imbibition, quantifying the contribution ratio of displacement/imbibition to recovery and revealing the combined oil recovery mechanism of displacement and imbibition.
The results of CT online scanning pressurized imbibition experiments indicate that the imbibition distance along the parallel direction of the matrix core is 3.2 cm, with a recovery rate of 9.40%. For the fracture core, the imbibition distance increased longitudinally along the parallel fracture surface direction, with a recovery rate of 19.36%. After imbibition, the volume of the fracture core increased by 1.5%, indicating that fractures can effectively enhance imbibition recovery. The opening of microfractures can significantly increase the permeability of the formation, providing substantial insights for optimizing oilfield production strategies.Results from the integrated displacement-imbibition experiments reveal that the contribution ratio of displacement in the core is 70.18%, with the primary utilization of medium-sized pores, while the contribution ratio of imbibition is 29.82%, with the primary utilization of micropores. Both sets of experiments demonstrate that pressurized imbibition plays a significant role in the combined recovery process of reservoir displacement and imbibition. The fracture zone is identified as the primary region where pressurized imbibition occurs in the oilfield.
This study systematically unveils the imbibition patterns within the matrix and fracture zones of tight oil and gas reservoirs, providing detailed measurements of the ranges and contributions of displacement/imbibition. These findings offer profound and specialized insights into understanding the reservoir energy storage mechanisms associated with hydraulic fracturing and optimizing oilfield production strategies.

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Poster / 553

The Crushing Characters of Quartz Sand Based on a New Experimental Image Processing Methods

Author: liansong Wu[1]

Co-authors: jianchun Guo ; xiaopeng Chen ; yutong Wu ; yuxuan Liu [1]; ziyi Peng

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Hydraulic fracturing has gradually increased as an important means to enhance production in deep low permeability reservoirs. Whether proppant can maintain long-term high conductivity in fractures has become a hotspot. Quartz sand has been widely used due to its affordability and easy preparation. However, the strength of quartz sand is low. Under high closure stress, quartz sand is crushed, producing fine particles that reduce fracture width and permeability of sand piles, resulting in a rapid decrease in fracture conductivity. Therefore, it is crucial to study the fragmentation law of proppants under high closure stress. For the study of the fragmentation law of quartz sand, a lot of related experiments have been conducted both domestically and internationally, and quantitative methods such as screening method and laser particle size analysis have also been formed, but there are certain limitations. In this study, a new image processing-based quantitative method is developed to determine the compression proppant crushing rate. Compared with conventional screening methods to verify accuracy, this method can more quickly and efficiently quantify the proppant crushing rate. Subsequently, a crushing experiment of quartz sand was conducted using the proposed method, and the proppant crushing rate under different conditions was calculated. The influence of factors such as sand spreading concentration, particle size combination, and sand placement method on the proppant crushing rate was analyzed. The results of this analysis were consistent with previous studies, confirming the applicability of the proposed method. This research provides a theoretical foundation for hydraulic fracturing and optimization of sand placement in order to maintain long-term high conductivity in fractures.

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Poster / 556

Applications of pore network modelling in predicting the permeability in hydrate-bearing sediment

Author: Yongchao Zhang[1]

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Permeability plays a pivotal role in governing the fluid flow within hydrate-bearing sediment (HBS) and significantly influences the efficiency of natural gas production from hydrate reservoirs. However, the measurement of HBS permeability is challenging due to the complexities of maintaining phase equilibrium conditions during testing. This study focused on the sandy hydrate-bearing sediments and intended to elucidate the evolution of absolute and relative permeability as a function of hydrate saturation by the mean of pore network modelling. In the developed model, the hydrate formation process in the porous media is simulated incorporating two key sub-processes: hydrate nucleation and hydrate growth. We integrated various theories from hydrate kinetics, including the random nucleation theory, interface growth theory, Ostwald-Ripening effect, and pore water

activity theory, to control the hydrate formation process. For modeling fluid flow within the pore networks, we utilized the conductivity calculation method. The constructed pore network model was employed to analyze permeability variations within different pore networks. Simulation results from a series of regular networks demonstrated that the distribution of formed hydrate and the permeability of HBS are influenced by factors such as model dimension, hydrate nucleation fraction, and hydrate growth type. Further simulations based on CT images showed the changes of absolute permeability and gas-water two-phase permeability during hydrate formation within different sandy sediments. As a result of these simulations, we provided parameter ranges suitable for the application of the Masuda model in predicting absolute permeability in sandy hydrate reservoirs, as well as the Brooks-Corey model and van Genuchten model for predicting two-phase gas-water permeability. This study is hoped to bring new insights into the field of micro-scale seepage research within hydrate reservoirs.

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Poster / 557

Microscopic mechanism investigation of counter-current imbibition in tight reservoirs using the Lattice Boltzmann method

Authors: Rundong Gong[1]; Hangyu Li[1]; Junrong Liu[1]; Shuyang Liu[1]; Dengfeng Zhang[1]

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Tight oil reservoirs are typically developed through hydraulic fracturing to create a network of fractures, with counter-current imbibition between fractures and matrix playing a crucial role. However, during the counter-current imbibition process, as water displaces oil, it increases water saturation and leads to water blocking phenomena, resulting in reduced oil relative permeability and heightened flow resistance in the oil phase. The oil relative permeability is pivotal in determining the matrix's ability to elastically expel oil, rendering counter-current imbibition with both advantages and disadvantages. To quantitatively characterize the damage caused by counter-current imbibition in tight reservoirs, we employed the lattice Boltzmann method to simulate counter-current spontaneous imbibition in Jimsar tight rocks. We also introduced a novel method for assessing reservoir damage: the water-to-solid transformation method.

During counter-current imbibition, the water phase occupies the flow space of the oil phase, acting as a solid, consequently diminishing the oil's flow capacity. Given the challenge of calculating the

relative permeability of two phases during counter-current imbibition, we transformed the water phase into a solid phase to construct a new digital core. This transformation allowed for the computation of unidirectional permeability, which was then used to characterize the reduction in oil relative permeability during counter-current imbibition. The study elucidates that the reduction in oil relative permeability in the digital core of Jimsar during counter-current imbibition is limited, ultimately establishing a relatively stable oil flow channel. This method facilitates the evaluation of the effectiveness of counter-current imbibition in reservoirs, enabling the implementation of appropriate improvement measures. Furthermore, a comparison between counter-current and co-current imbibition indicates that the water phase in counter-current imbibition only affects the oil phase near the fracture, without reaching the interior of the matrix. Nevertheless, the imbibition front of counter-current imbibition remains relatively stable, without significant fingering.

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MS06-A / 558

Upscaling of Relative Permeability on a Laminated Sandstone after Pore-scale Rock-typing Using Minkowski Functionals

Author: Han Jiang[None]

Co-authors: Chaozhong Qin [1]; Christoph Arns [2]; bowen shi [3]

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Relative permeability is an essential parameter to describe flow and transport in porous media, which is a vital process throughout various underground engineering and environmental projects. Traditional laboratory measurements for two-phase flow in rock samples are rather time-consuming and financially expensive. Digital physical analysis, on the other hand, provides a convenient alternative with the assist of advanced X-ray imaging technology. Nevertheless, limited by computational resources, pore-scale numerical simulations are normally conducted on a homogeneous cubic digital sample with a side length of a few hundred voxels. For a highly resolved image, the physical size may even be smaller than a cubic millimeter, which is inadequate to serve practical purposes. Hence, upscaling of pore-scale numerical simulation to continuum scale has attracted extensive interest, which is challenged by severe structural heterogeneity of reservoir rock and the limitations on imaging and computational aspects. Towards the issue, we offer a novel approach of pore-scale rock-typing and relative permeability upscaling. Integral geometry is applied on a 3D segmented

tomogram of a laminated sandstone to compute regional Minkowski measures of volume, surface area, the integral of mean curvature and the integral of total curvature. The feature maps are then utilized for the recognition of relatively homogeneous regions/pore-scale rock-types through Support Vector Machine method. A few subsamples are then extracted from each rock-type to compute the representative capillary pressure and relative permeability curves using Pore Network Model, which are assigned back to corresponding regions of the rock-type distribution map before fast upscaling of the whole image applying van Genuchten model. The upscaling results are then compared with full-scale computation on the original tomogram. The excellent agreement has indicated great potential of this approach to bridge the gap between pore-scale and continuum-scale two-phase flow research under the guarantee of accuracy and computational efficiency.

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MS03 / **559**

A new model for predicting conductivity under nonlinear fracture closure and proppant crushing grading curve evolution

Author: liansong Wu[1]

Co-authors: jianchun Guo ; simin He ; yutong Wu ; yuxuan Liu

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To solve the problem of rapid decline in conductivity of sand filled fractures in deep shale, based on the mechanical process of compression and deformation of proppant pile, the constitutive equation of deformation and fracture of proppant pile was established, and the transfer matrix of gradation curve after fracture of proppant pile was established based on fractal theory. Combined with KC equation, the equivalent particle size and permeability evolution equation of sand pile under multi-particle fracture were deduced. Finally, a new model for predicting the conductivity of proppant embedment deformation and fracture is obtained. The new model is compared with the results of fracture width deformation experiment, sand pile permeability experiment and multi-particle size combination conductivity experiment, which proves the correctness of the model. The results show that the change of net closing pressure will change the fracture width and permeability, and thus change the fracture conductivity. The dominant factor of the change of conductivity is the net closing pressure, and the greater the net closing pressure, the smaller the conductivity. The main factor affecting the change rate of fracture width is the apparent elastic modulus of proppant pile. The larger the apparent elastic modulus is, the larger the fracture width is. The main factor affecting the change rate of fracture permeability is the fracture degree of proppant pile. The larger the fracture degree is, the smaller the permeability is. The larger the combination ratio of large particle size, the higher the conductivity. Therefore, the development of proppants with high apparent elastic modulus and low degree of breakage is of great importance to improve the conductivity. At the

same time, this model also improves the theoretical guidance for proppant particle size combination selection, which is helpful to the optimization design of field construction.

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Study on Ct Online Pressurized Imbibition and Numerical Simulation of Tight Sandstone

Authors: Yanan Zhang[1]; Yuliang Su[None]; Guanglin Yu[None]; Wendong Wang[None]

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Due to the extremely low permeability and underdeveloped porosity in tight oil and gas reservoirs, efficient development of tight oil reservoirs typically necessitates hydraulic fracturing to establish industrial productivity. Pressurized imbibition processes, induced by pressure differentials and capillary forces, persistently occur within the matrix and fractures, playing a pivotal role in oil-water displacement. Through CT online scanning, pressurized imbibition experiments, and simulations, the imbibition processes under pressure have been characterized, delineating the range of pressurized imbibition within tight oil reservoirs. These findings provide guidance for selecting the optimal shut-in well imbibition time, contributing valuable insights for the effective development of tight oil reservoirs.

In this study, real matrix and fractured core samples from tight reservoirs were utilized to conduct CT online scanning pressurized imbibition experiments. By real-time observation of the pressurized imbibition behavior of matrix and fractured cores, the pressurized imbibition distances of the two types of cores were determined, revealing differences in recovery rates under varying conditions. In the numerical simulation section, control equations under two-phase oil-water flow conditions were coupled to establish a one-dimensional mathematical model for pressurized imbibition in tight rock cores, considering capillary forces and osmotic pressure. Fitting the recovery rates and imbibition distances for pressurized imbibition in the cores, we determined the optimal shut-in well imbibition time under different injection pressure conditions. This provides concrete time references for engineering decisions, facilitating the enhancement of production efficiency and the optimization of reservoir development strategies.

The experimental results indicate that the matrix core exhibits imbibition along the parallel direction, with a imbibition distance of 3.2 cm and a recovery rate of 9.40%, without any breakthrough phenomenon. In contrast, the fractured core experiences inward imbibition along the parallel fracture plane, with a slightly increased longitudinal imbibition distance and a recovery rate of 19.36%. Water rapidly moves through the fracture, resulting in a swift water breakthrough, and the fractured core's volume increases by 1.5% after pressurized imbibition. This suggests that fractures effectively

enhance imbibition recovery rates, and the opening of micro-fractures significantly improves reservoir permeability, providing substantial insights for optimizing oilfield production strategies. Utilizing a one-dimensional pressurized imbibition numerical simulation model, the recovery rate and imbibition distance of the matrix core under pressure imbibition were fitted, yielding an optimal shut-in well imbibition time of 300 hours. The shut-in well time optimized through this simulation method can provide necessary references for engineering decisions.
This study systematically and deeply reveals the imbibition law of matrix and fracture region in tight oil and gas formations, and provides profound professional insights for understanding the mechanism of energy storage in braised Wells and optimizing oilfield production strategies.

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Poster / 562

The influence of matrix lower limit on structure and flow characteristics in tight oil reservoir

Authors: Chenchen Wang[1]; Denglin Han[1]; Rongrong Hu[1]; Hao Du[1]; Miaomiao Su[1]

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The formation space of tight oil reservoir is complex, which develops both matrix pores and microfractures, and the classification of matrix pore lower limit has an important influence on the structure and flow characteristics of tight oil reservoirs. In this paper, CT scanning method is used to acquire representative 3D grayscale images of matrix and micro-fracture samples in tight oil reservoir respectively, and the corresponding matrix pore and micro-fracture network models are extracted by the maximal ball method. Based on the matrix pore and micro-fracture network models with the same physical size, network superposition method is introduced to construct the tight oil reservoir network models by adding virtual connected throats, and the superimposed network could contain the structural characteristics of both matrix pores and microfractures. By setting different lower limits of matrix pore diameters, the matrix pore network with different lower limits are developed and the corresponding tight oil superimposed networks are constructed. It can be found that, as the lower limit of matrix pore diameter increases, the distribution curves of pore and throat diameter in matrix system keep shifting to the right, the average coordination number keeps decreasing, which shows poor connectivity. The contribution of matrix system to formation total porosity slightly decreases but does not change much, the contribution of matrix system to formation total permeability keeps decreasing; the imbibition relative permeability curve of oil phase keeps shifting to the right, and the imbibition relative permeability curve of water phase keeps shifting to the left, and the oil-water co-flow zone keeps decreasing.

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MS08 / **565**

A mechanistic investigation of oscillatory zoning using reactive transport modeling

Author: Hang Deng[1]

Co-author: Jenna Poonoosamy

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Solid solutions are widely studied because their formation is ubiquitous in natural and anthropogenic systems. Co-precipitation in rock matrix can result in oscillatory zonation phenomena with solid solutions exhibiting compositional variations (e.g., plagioclase). The principle of co-precipitation of sulphate solid solution is relevant for wastewater treatment of produced waters from hydraulic fracturing and oil/gas extraction, for removing contaminant in uranium mines etc. For nuclear waste disposal, the formation of solid solutions is considered as an important retention mechanism for 226Ra. Despite the widespread occurrence of solid solutions and well-established thermodynamic models, their formation in rock matrix and the effects of transport and kinetics are poorly understood. Previous microfluidic experiments of diffusion-controlled precipitation showed patterns of oscillatory zoning of solid solution crystals of (Ba,Sr)SO4 1. In this study, reactive transport modeling is performed to provide a mechanistic understanding of the oscillatory zoning behavior. A micro-continuum approach based reactive transport model that considers probabilistic nucleation was used to simulate the precipitation of (Ba,Sr)SO4 solid solutions following the experimental geometry and setup 2. It enabled us to compare the contributions of physical-chemical processes that include species-specific diffusion at the solid-fluid interface, solubilities, nucleation kinetics and crystal growth. The models have highlighted that reaction kinetics, rather than transport, are more important in shaping the oscillatory zoning phenomena.

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2. Deng, H., J. Poonoosamy, and S. Molins, A reactive transport modeling perspective on the dynamics of interface-coupled dissolution-precipitation. Applied Geochemistry, 2022. 137: p. 105207.

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MS03 / **566**

Investigating interface coupled mineral dissolution and precipitation processes using advanced analytical and modelling tools

Author: Jenna Poonoosamy[None]

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Interface-coupled dissolution and precipitation (ICDP) 1 occur in various subsurface applications, e.g., serpentine carbonation in the context of CO2 sequestration, the carbonation of concrete causing degradation, anoxic steel corrosion in geological disposal facilities for nuclear waste, or during groundwater remediation using permeable reactive barriers. ICDP is characterized by the dissolution of a primary mineral and the precipitation of a secondary mineral on its surface (rim formation). The precipitated secondary minerals can either develop porosity and fractures that enable fluid exchange and thereby completely replace the primary minerals or shield/ passivate them. Therefore, understanding the factors that regulate the development of the rim is critical for predicting the geochemical reactions and the resulting impacts on various geological and environmental systems over geological time scales. To this end, we developed a column experiment where we investigated the dissolution of celestine followed by the precipitation of barite 2. This is a well-controlled chemical system that is neither pH- nor redox-sensitive. The theoretical models to describe passivation processes in our experiment (e.g., Daval et al., 2) were simplified and did capture the underlying processes [3]. Micro-continuum modelling work showed that the porosity of the precipitates could play a secondary yet significant role in shaping the evolution of the co-dissolution and precipitation interface [5]. Currently, we investigate the micro and nano porosity of the secondary mineral using 3D FIB-SEM and evaluate the effective diffusivity in the precipitates using pore-scale modeling [6]. In addition, we conduct complementary microfluidic experiments combined with in-situ Raman 2D/3D and modelling to evaluate the effect of fluid velocities and solution saturation ratio (Peclet number and Damköhler number) with respect to the barite overgrowth thickness. These investigations will enable the identification of parameters that control or limit passivation and its associated potential effects on further mineral reactivity.

1 Renard et al., Timescales of interface-coupled dissolution-precipitation reactions on carbonates, https://doi.org/10.1016/j.gsf.2018.02.013
2 Poonoosamy et al., Combination of MRI and SEM to Assess Changes in the Chemical Properties and Permeability of Porous Media due to Barite Precipitation, https://doi.org/10.3390/min10030226
[3] Daval et al., Carbonation of Ca-bearing silicates, the case of wollastonite: Experimental investigations and kinetic modelling, https://doi.org/10.1016/j.chemgeo.2009.01.022
[4] Poonoosamy et al., Effects of solution supersaturation on barite precipitation in porous media and consequences on permeability: Experiments and modelling, https://doi.org/10.1016/j.gca.2019.11.018
[5] Deng et al., A reactive transport modeling perspective on the dynamics of interface-coupled dissolution-precipitation https://doi.org/10.1016/j.apgeochem.2022.105207

[6] Yang and Wang, Pore-scale modeling of chloride ion diffusion in cement microstructures, https://doi.org/10.1016/j.cemconco

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MS01 / **568**

Towards an open-source digital twin for subsurface geothermal systems: a proof-of-concept study for a doublet system

Author: Guofeng Song[1]

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Geothermal energy can provide clean and sustainable baseload energy for heating, cooling, and power. The injected working fluid undergoes flow and heat transfer within the surrounding porous rocks during the geothermal reservoir extraction. The geological complexity and lack of data require digital technology like computer simulation to assist in the optimization and decision-making of operation strategies. A digital twin denotes a virtual representation of a physical product, process or facility, and is used to understand and predict the physical counterpart's performance. A digital twin for geothermal production can help to mitigate operational risks, reduce maintenance costs, extend reservoir longevity, and enhance overall sustainability of a geothermal resource.

We propose a workflow for an open-source digital twin for geothermal energy that contains the following elements: a) Well logs and seismic data are utilized to design multiple reservoir models that capture possible geological scenarios using the Rapid Reservoir Modeling (RRM) software. RRM is a sketch-based modelling software that allows users to rapidly sketch geologically consistent models in 3D. b) Possible property distributions will be assigned to geological domains to capture uncertainty in the petrophysical data. c) The Delft Advanced Research Terra Simulator (DARTS) is combined with machine learning techniques to create proxy models that enable fast simulations. d) As new production and monitoring data becomes available, data assimilation techniques like Ensemble Smoother with Multiple Data Assimilation (ESMDA) are applied to update property distributions for each scenario. This iterative process of data assimilation will help users constrain geological and production uncertainties, both of which are key to optimizing operational strategies.

We demonstrate the digital twin framework using a proof-of-concept study of a low-enthalpy geothermal system located in a channelized fluvial reservoir. Heat is produced from a geothermal doublet. The geological scenarios were designed using RRM. These models consider key uncertainties, such as Net to Gross, sinuosity of the channels, paleo flow direction, and the distribution of porosity and permeability within the geological domains. One of the RRM models was chosen to be the "truth case"for which synthetic production data (well temperatures and pressures) and dynamic data along

the wells were simulated using DARTS. Each individual RRM model adheres to the well constraints "observed"for the truth model. DARTS was applied to rapidly predict production performance for each scenario, and these data can subsequently serve as the training set to obtain the proxy model. Both machine learning and ESMDA will be performed to reduce the difference between the prediction and observation of truth case to update reservoir properties.
The outcomes of this proof-of-concept study demonstrate the feasibility of the digital twin framework for geothermal systems. A broader range of monitoring data in the reservoir and transient data will be included in the future to enhance the performance of the digital twin in geothermal energy applications.

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MS11 / 569

Pore-scale morphologies of CO2 hydrate formation in microfluidics with in-situ Raman spectroscopy for CO2 sequestration

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CO2 hydrates are cage-like solid compounds consisting of CO2 gas molecules and water molecules. The properties of CO2 hydrates, such as high gas storage capacity and moderate formation conditions of pressure-temperature, are desirable for long-term and safe CO2 storage in geological setting. The purpose of work is to probe the feasibility of CO2 storage in hydrate in marine subsurface. Compared to natural gas hydrates, it is difficult to investigate morphological CO2 hydrate dynamics in microfluidics, as the morphologies of CO2 in liquid and water phases are similar. In this work, two scenarios were investigated regarding different CO2 states controlled by different pressures above or below CO2 liquid liquefaction pressure (PL-CO2), by means of pore-scale microscopic observation coupled with in-situ Raman spectroscopy in microfluidic chip. In one scenario, the system pressures were kept lower than PL-CO2 to form CO2 hydrate. The system was tested by both microscope and Raman spectroscope to distinguish CO2 in gas, water and hydrate. A pressure difference was observed in the system indicating hydrate blocked pore channels and prevented unwanted CO2 flow. In another scenario, the system pressures were increased over PL-CO2, which was the typical reservoir pressure, to observe CO2 hydrate formation in the system containing liquid CO2. The differences between both morphological patterns and Raman peak shift were observed, verifying CO2 could be stored in states of both hydrate and liquid. The quantitate calculation of CO2 storage capacity showed about 80 volumes of CO2 was retained in the system having only CO2 hydrates, compared with about 150 volumes of CO2 stored in the system having both CO2 hydrates and liquid CO2. The morphological patterns, Raman spectra and calculation of storage capacity indicates that

CO2 hydrate storage could serve as a secondary storage option for geological CO2 storage in marine subsurface. The results of this work are beneficial to understand marine CO2 hydrate storage in confined space of porous media, and the enhanced CO2 hydrate storage capacity can be explored by coupling with hydrate promotors and thus achieve more efficient CO2 storage in marine subsurface conditions.

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MS15 / 574

Efficient Surrogate Modeling of Subsurface Flow in Porous Media Using Transfer Learning with Multifidelity Data

Author: Jiawei Cui[1]

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ABSTRACT
In subsurface flow settings, deep-learning-based surrogate modeling is shown to be an effective approach to deal with cases that require a substantial amount of model simulations. However, a large number of high-fidelity training simulations are usually required to construct these deep-learning-based surrogate models. For large-scale models, it can be computationally prohibitive to perform these training simulations. To address this limitation, in this work, we develop a new approach to construct surrogate models using transfer-learning with multifidelity training data. The model is based on a U-Net deep-learning architecture, wherein we introduce a specialized input layer, in order to allow for gradual model fine-tuning with multifidelity data, and an embedded layer that is designed to deal with time-varying source/sink terms. The procedure of building such surrogate models can be divided into three steps. In the first step, a relatively large amount of low-fidelity simulations, generated from upscaled coarse models, are used to build a pre-trained deep-learning model. In the second and third steps, the input, output, encoder, embedded, and decoder layers of the model are progressively fine-tuned, requiring a relatively small number of high-fidelity simulations. In this study, we use 400 low-fidelity and 100 high-fidelity training simulations, which leads to about a 70% reduction in computational cost of the overall procedure. The proposed procedure is applied to three cases with different number and locations of source/sink wells. In all cases, our proposed surrogate models trained using multifidelity data provide predicted dynamic pressure and saturation fields that are in close agreement with the corresponding model trained using only a large number of high-fidelity data. In addition, our introduction of the embedded layers is shown to effectively

improve the prediction accuracy of the surrogate model when dealing with time-varying source/sink well terms, in comparison with traditional approaches based on similar network architecture.

Keywords：Subsurface Flow Simulation; Porous Media; Surrogate Model; Transfer Learning; Multi-fidelity Training Data;

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Poster / 577

The Competitive Adsorption Behavior of CH4/CO2/H2S Mixtures in Kerogen Nanopores from the Perspective of Molecular Simulation

Author: Junyao Bao[1]

Co-authors: Shaofeng Ning [1]; Jingkai Cui [1]; Shiyuan Zhan [1]; Xiaoguang Wang [1]

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Objectives/Scope:
*Nowadays, the escalating greenhouse effect is primarily attributed to the excessive emissions of CO2. Geologic sequestration of CO2 and the utilization of CO2 in displacing shale gas during gas production process could be benefit for mitigating CO2 levels. The presence of H2S gas in CO2 waste emissions often poses a challenge due to the potential cost escalation associated with its purification. In response to this, the concept of CO2/H2S co-sequestration has been proposed, with successful implementation cases reported. However, the application of CO2/H2S displacement in shale gas extraction has yet to be verified. In this work, we used the Grand Canonical Monte Carlo (GCMC) method to simulate the adsorption of different components (CH4, CO2, H2S in single-phase, CH4:H2S=1:1 in two phases, and CH4:CO2:H2S=5:4:1 in three phases) within kerogen at 373.15K under various pressures. The study investigated the adsorption density, adsorption capacity, and competitive selectivity adsorption coefficients of different components on the kerogen surface. Our works could reveal the adsorption patterns of CH4/CO2/H2S in kerogen pores, providing a theoretical foundation for the injection and extraction of shale gas with CO2/H2S.*Methods/Procedures/Process:
Adsorption behavior in ~5nm kerogen nanopores with different components systems is investigated at 373.15K and a series of pressures. The CVFF, TraPPE-EH, TraPPE-UA, and three-point potential models are used to describe the kerogen nanopores, CO2, CH4, and H2S, respectively. All the GCMC simulations are completed by the MCCCS Towhee software. In the μVT ensemble, 5000000 steps per fluid molecule are carried out to achieve equilibrium, and 10000000 steps per fluid molecule are conducted for sampling. Based on statistical data, we calculated the accessible volume, adsorption

density, adsorption capacity, and competitive selectivity adsorption coefficients.
Results/Observations/Conclusions:
*It was observed that CO2 effectively reduces the adsorption of CH4, but the introduction of H2S significantly decreases the adsorption density of CO2, while the adsorption density of CH4 remains essentially unchanged. The isothermal adsorption curves reveal that the injection of both CO2 and CO2/H2S leads to a reduction of approximately 50% in the adsorption quantity of CH4, indicating effective shale gas extraction. In systems with the addition of H2S, the adsorption quantity of CO2 decreases by around 30% compared to systems with only CO2 injection. The competitive adsorption coefficients of CH4 relative to other components in different systems are all less than 1 and range between 0.2 and 0.4, suggesting a strong adsorption capacity of kerogen for both CO2 and CO2/H2S.*Applications/Significance/Novelty:
This work reveals the adsorption patterns of CH4/CO2/H2S in kerogen pores from a molecular perspective and provides crucial insights into the competitive adsorption patterns of CH4, H2S, and CO2, which is helpful to lay a theoretical foundation for the simultaneous injection and extraction of shale gas with CO2/H2S.

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Poster / 578

Effect of catalyst particle size distribution in the catalytic layer on the performance of water electrolysis in proton exchange membrane pore scale simulation

Author: Jiaxin He[1]

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In this study, the effect of catalyst particle size on the performance of proton exchange membrane water electrolyzer (PEMWE) was studied by using the Lattice Boltzmann Method (LBM). The results show that compared with the catalyst particle distribution, the catalyst particle size is the main factor affecting the performance of the catalytic layer of the anode. Homogenized catalyst particles with smaller particle size can effectively increase the specific surface area of catalyst particles and increase the ECSA of the catalytic layer, thereby improving the electrochemical reaction performance of the catalytic layer. the electrochemical performance of the catalytic layer can be effectively improved by using catalyst particles with smaller particle size and more uniform distribution in the preparation of the catalytic layer (the average local reaction current is 0.13A/cm2 at 3V)
This study investigates the effect of catalyst particle sizes on the performance of a PEMWE using the lattice Boltzmann method (LBM). The findings reveal that the size of catalyst particles plays a crucial role in determining the performance of the anode CL, surpassing the influence of catalyst particle size distribution. Utilizing smaller and more uniform catalyst particles enhances the specific surface area and electrochemical reaction performance of the CL.
Key words: PEMWE, LBM, Catalyst layer, Gaussian distribution

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1 Mohd Alam, Kuldeep Kumar, Saket Verma, Viresh Dutta, Renewable sources-based DC microgrid using hydrogen energy storage: Modelling and experimental analysis, Sustainable Energy Technologies and Assessments, Volume 42,2020,100840, ISSN 2213-1388,

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MS09 / **579**

A Benchmark Study of Pore-scale Multiphase Flow in Pore-doublet: The Impacts of Hydrodynamics on Mineral Dissolution Reaction Rate

Author: Xin Wang[1]

Co-authors: Rixuan Wang [1]; Hang Deng [1]

[1] *Peking University*

Corresponding Authors: hangdeng310@gmail.com, 2000011076@stu.pku.edu.cn, alanxin@stu.pku.edu.cn

Abstract: Multiphase flow in porous media is ubiquitous in soils, oil and gas reservoirs, geologic carbon storage and hydrogen storage systems, and batteries. In recent years, direct observation using microfluidic experiments and pore-scale numerical modeling have become increasingly important tools for studying pore-scale fluid dynamics. To further examine the precision of the experiment and

evaluate the performance of numerical models in order to expand beyond experimental conditions, it is necessary to develop proper benchmark experiments.
emsp;emsp;In this work, a benchmark study is developed for gas-water two-phase flow through a pore-doublet geometry. Microfluidic experiments for a range of capillary numbers and fluid properties were performed and characterized using optical microscopy techniques. Subsequently, the experiments were numerically simulated using the interFoam and interFlow solvers in OpenFOAM, and the phase-field and level-set methods in COMSOL. The comparison enables us to systematically examine the impacts of modeling decisions (e.g., mesh resolution, model dimensionality) under a range of flow rates and wettability conditions. Finally, mineral dissolution was numerically simulated using CrunchFOAM, a solver based on OpenFOAM and coupled with the CrunchTope geochemical framework, to evaluate the subsequent impacts on geochemical reactions in two-phase systems.

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Poster / 580

Multi-scale Pore Structure Characteristics of Deep Marine Shale and Its Controlling on Gas Transport Mode: Silurian Longmaxi Formation in Southern Sichuan, China

Author: Shijie He[1]

Co-authors: Pingping Li [1]; Xianglu Tang [1]; Zhenxue Jiang [1]

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The attributes of shale pore structure govern the accumulation, presence, and dissipation of gas. Deep marine shale undergo intricate geological evolution, with pore development at the nanoscale. Consequently, quantifying the impact of deep shale pore structure on gas is challenging. In this paper, the microscopic storage space structure of deep shale is quantified, and the correlation between pore structure and mode of gas transport is established. The study focused on the Silurian Longmaxi Formation shale, utilizing techniques such as SEM, CO2 and N2 adsorption, HPMI, and the Frenkel-Halsey-Hill method approach to quantify the development characteristics and controlling factors of pores at multiscale. Based on the pore structure, fractal, and molecular dynamics of methane, the numerical correlation linking pore structure and gas transportation mechanisms was established. The results indicate that the deep marine shale formations are predominantly composed of ORSS and ORMS. The evolution of pores is impacted by the TOC content and mineral composition. Based on the governing function of pore structure in gas transport mechanisms, the pores can be classified into three categories: ultramicro adsorption pore, nano-diffusion pore, and micro-nano

flow-diffusion pore. Correspondingly, there are five types of gas transport modes: surface adsorption diffusion, Knudsen diffusion, Fick diffusion, slip flow, and continuously flow. These diverse modes collectively form a complex gas transport network. Deep shale exhibits a greater abundance of micropores and mesopores compared to shallow shale. The contribution of micro-fractures to shallow shale gas transport is crucial, and the contribution to deep shale decreases significantly. In conclusion, the favorable exploration lies in targeting ORSS formations with low D1 (fractal dimension) and high D2 (fractal dimension), as well as ORMS segments with high D1 and high D2. Specifically, within hydrocarbon-rich basins located below 3500 m, it is recommended to search for overpressure regions with weak structural deformation. These areas hold potential for successful gas exploration. This research establishes a basis for the exploration, development, and geological principles of deep shale gas.

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Poster / 581

Investigation of fault damage zones from direct shear tests and implications for hydraulic fracturing process

Author: Zifang Zhu[1]

Co-authors: Shengwen Qi [1]; Weiwei Zhu [1]; Bowen Zheng [1]

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Hydraulic fracturing is an important stimulation technique for extracting resources from low-permeable formations. Apart from hydraulic fracturing (where pore pressure exceeds the minimum principal stress), hydraulic shearing (where pore pressure does not exceed the minimum principal stress) is an essential mechanism in forming the stimulated reservoir volume and controlling the ultimate stimulation results, especially for shale formations with layered beddings (Li et al., 2019). Shear failure in rocks will not only generate primary fractures but also cause stress alteration in the neighboring region around the primary fracture. Such stress alteration affects the rocks' stability and possibly induces more secondary fractures. This phenomenon is also known as fault damage zones, commonly observed in rock masses at different scales (Kim et al., 2004; Sui et al., 2019). In reality, it is almost impossible to directly observe the shear failure process in the subsurface. Therefore, in this work, we adopted an advanced dynamic direct shear testing device to break rocks (Qi et al., 2020) and a micrometer CT to observe the fault damage zones after the shear failure. Quantitative descriptions of the damage zone, such as fracture intensity, roughness, and connectivity, are summarized.
In this research, an independently designed dynamic direct shear testing device (Qi et al., 2020) was utilized to conduct in-house direct shear tests on layered shale specimens with various layer

angles (0°, 30°, 45°, and 60°). Subsequently, the sheared shale specimens were scanned with a micrometer CT, and 3D digital cores were reconstructed. Fine segmentation of micron-scale fractures in inhomogeneous shale was achieved using multiple processing algorithms. Considering different bedding structural surfaces, the physical properties and geometrical features of 3D micrometer-scale fractures in shale were quantitatively evaluated. Parameters such as fracture density, 3D shape factor, roughness, Euler number, and morphological filtering were employed to subdivide the damage zones along the main fracture surface.
From the preliminary results, we divided the generated fractures into three categories based on their spatial distribution: the primary induced fracture, fractures in the connected damage zone, and isolated fractures. The range of damage zones varies significantly with different bedding angles. With the increase in bedding inclination, the density of fine fractures distributed along the primary shear fractures initially increases and then decreases, reaching the maximum in samples with 30°inclined layers. The roughness of primary fracture surfaces and secondary fractures in shale samples with different bedding angles displays significant anisotropy and asymmetry, with greater roughness observed at the microfractures and fractures in connected damaged zones. Morphological patterns of the three types of fractures are further discussed. An in-depth understanding of the fault damage zone provides valuable insights to evaluate and optimize the hydraulic fracturing process.

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MS03 / 582

Rigorous Derivation of Discrete Fracture Models for Darcy Flow in the Limit of Vanishing Aperture

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We consider single-phase flow in a fractured porous medium governed by Darcy's law with spatially varying matrix-valued hydraulic conductivities in both bulk and fractures. In particular, we account for general fracture geometries parameterized by aperture functions on a submanifold of codimension one. Given a fracture with a width-to-length ratio of the order of a small parameter ε, we derive

limit models as $\varepsilon \to 0$. In the limit $\varepsilon \to 0$, we obtain discrete fracture models where fractures are represented as submanifolds of codimension one. The limit models provide a computationally efficient description with explicit fracture representation, while avoiding thin equi-dimensional subdomains with a need for highly resolved meshes in numerical methods. The ratio $K_{\mathrm{f}}^{\star}/K_{\mathrm{b}}^{\star}$ of the characteristic hydraulic conductivities in the fracture and bulk domains is assumed to scale with ε^{α} for a parameter $\alpha \in \mathbb{R}$. Depending on the value of α, we obtain five different limit models as $\varepsilon \to 0$, for which we present rigorous convergence results. Additionally, preliminary results are also available for the case of two-phase flow.

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MS03 / **583**

Experimental and molecular simulation studies of methane adsorption on deep shales

Author: Weijun Shen[1]

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Understanding methane adsorption behavior on deep shales is crucial for estimating the original gas in place and enhancing gas recovery in deep shale gas formations. However, the methane adsorption behavior on deep shales under high pressure is challenging, and many uncertainties still exist in the process. In this study, the methane adsorption on deep shales within the Lower Silurian Longmaxi Formation from the Sichuan Basin, South China were conducted at pressures up to 50 MPa. The effects of total organic carbon (TOC), temperatures, clay minerals and moisture content on the adsorption capacity were discussed. Then the molecular models of kerogen nanopores with different shapes and sizes were constructed based on kerogen structure unit of deep shale from the Longmaxi Formation, and the methane occurrence were conducted by coupling a grand canonical Monte Carlo algorithm and a molecular dynamics algorithm. The results indicated that the methane excess adsorption on deep shales increased, then reached its peak and finally decreased with the pressure. The methane adsorption capacities exhibited strong positive correlations with the TOC content and negative relationships with clay minerals. The methane excess adsorption decreased as the temperature while the opposite trend would occur once it exceeded some pressure. The presence of the moisture content on deep shales sharply decreased the methane adsorption capacities, and the reduction of the adsorption capacity decreased with the pressure. The methane adsorption capacity in deep shales is negatively correlated with temperature, and high temperature will inhibit the affinity of methane molecules in pores.

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MS22 / 584

New insights in battery electrolyte behavior during cycling and heating of batteries using dynamic micro-CT

Author: Wesley De Boever[None]

Co-authors: Jan Dewanckele [1]; Ksenija Nikolic [2]; Marijn Boone [1]; Zachary Karmiol [3]

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In this work, we present unique results of dynamic micro-CT to study the behavior of Li-ion batteries during two important events that determine battery quality and lifetime. First, we show the interactions between different battery components during the first few charge and discharge cycles of a battery, the so-called formation cycles. How these cycles are performed has a huge impact on the lifetime, capacity, and overall quality of Li-ion batteries. During these cycles the solid-electrolyte-interface (SEI), a thin layer on the surface of the electrode material, is formed. This SEI is formed by the reaction between the electrode and the electrolyte and serves as a layer where Li+ ions can be embedded and removed during further cycling of the battery. This makes optimizing the formation cycles one of the most important research topics in battery production. Since the SEI is very thin (100 nm), high-resolution methods such as (FIB)SEM are used to study it. Although dynamic micro-CT cannot visualize the actual SEI layer, it can be used to visualize 3D electrolyte movement in real time and study swelling and shrinking of the entire battery during cycling. For the experiment, 15 x 25 cm large pouch cells were pressurized and mounted in the TESCAN DynaTOM, a unique micro-CT system with a rotating gantry to allow for complex in-situ experiments. Using an externally controlled potentiostat, several charge and discharge cycles were programmed with specific charging speeds, and several high-quality static (60 minutes per scan) and fast dynamic (2 minutes temporal resolution) micro-CT scans were performed at 13 predetermined intervals during the 28-hours procedure. In this work, we show results on 4D electrolyte movement, gas formation and structural dynamics in these pouch cells.

In a second experiment, the behavior of cylindrical cells under increased temperatures was observed. Elevated temperatures as low as 60 ℃ already have a negative effect on lifetime and will result in degradation and irreversible damage. To observe the structural effect of increased temperatures, a 26650 cell was heated up to ~60 ℃ using Peltier elements powered through the slipring of the scanner's rotation stage. In a series of dynamic and time-lapse micro-CT scans, the movement of the

electrolyte in and out of the electrode layers was observed in 3D. Novel machine learning protocols enable segmentation of the different battery components (cathode, anode, electrolyte, and gas) and follow their movement over time. In further experiments, the effect of higher temperatures, and faster or longer heating will be examined.

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MS21 / 586

Universal scaling law of bubble dissolution in porous media

Author: Yuehongjiang Yu[None]

Co-author: Ke Xu [1]

[1] *Peking University*

Corresponding Authors: 2101112003@pku.edu.cn, kexu1989@pku.edu.cn

Dissolution of bubbles in porous media affects many important geological and engineering processes, such as CO_2 sequestration, hydrogen storage, fuel cell water management and Li-battery electrolyte filling. However, although dissolution of continuous gas phase has been investigated extensively, there is still no universal theory for static bubble dissolution kinetics in porous media. We thus conduct experimental and theoretical investigation on the universal dissolution theory for bubbles in porous media.

We found that porous structure does not only change the effective diffusivity, but also regulate the characteristic mass transfer distance and surface area. In open space, the mass transfer area (S) of the bubble is the surface area of the bubble itself, and the characteristic mass transfer distance is proportional to the bubble radius R 1. These result in V~t scaling in 2-d and $V^{2/3}$~t scaling in 3-d in quasi-steady state, where V is the dissolved volume. However, in porous media, both its mass transfer area and its characteristic mass transfer distance are re-regulated by the porous structure. The concentration in the pore body is almost uniform, while the concentration gradient is concentrated along the throat (Fig.1a). Consequently, the characteristic mass transfer distance is determined by throat length (L_t), and effective mass transfer area is determined by the throat cross section area (A_t) and available number of throats (n).

For a bubble in a single pore, n is a constant, resulting in a linear V~t scaling. For a large bubble that occupies many pores, n depends on the shape of the bubble. If the bubble is completely liner, n is proportional to the volume of the bubble V, so we can deduce lnV~t. While if the bubble is a bulk, n^2 is proportional to V, leading to a $V^{1/2}$~t scaling. These conclusions have been well verified by experiments. (Fig.1b).

In addition ,we investigate the dissolution of CO_2 bubble in porous media under gravity field, where the Rayleigh-Darcy convection can be induced in the liquid phase as dissolved CO_2 increases water

density. In case that the mass transfer is dominated by convection, the bubble dissolution rate becomes proportional to the flux of fresh water through the bubble. For an isolated CO_2 bubble in an infinitely-large porous medium, the flux is determined by the number of pores it occupies perpendicular to the gravitational field n_vert. Therefore, for a CO_2 bubble in a single pore (Fig.1c), the dissolution is in constant rate (V~t), that is experimentally examined.
In summary, we establish the scaling laws for bubble dissolution in porous media. We show that bubble dissolution kinetics in porous media becomes very different from that in bulk, not only in the value of diffusivity, but (more significantly) also in the volume-time scaling, because porous structure regulates the mass transfer length and area.

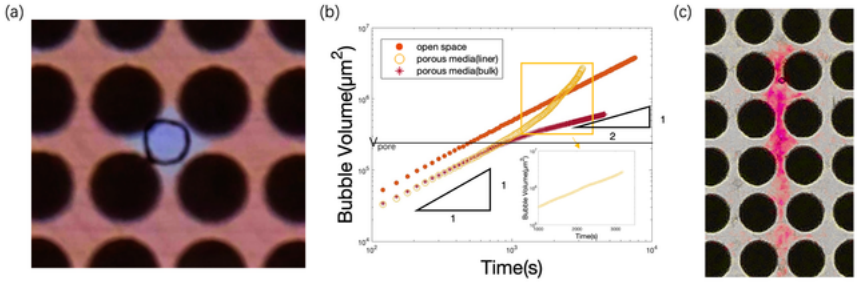

Figure 8: (a) The concentration field of dissolved bubbles in a single pore （b）Data on the volume of bubble dissolution over time under different conditions（c）The concentration field in which a bubble dissolves in a gravitational field

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589

A novel deep learning-based automatic workflow for multi-field coupled surrogate flow models

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The exploration of resources beneath the surface involves complex physical processes that require a significant amount of computational time and cost when using traditional numerical approaches. However, recent advancements in deep learning have led to the development of surrogate flow models that can significantly accelerate these processes by accounting for about 1000 times or more. Previous studies have mainly focused on oil drive or CO2 storage cases that lack thermal fields or chemical reactions, ignoring multi-field coupled flow problems. In this study, we propose a novel deep-learning-based surrogate flow model that can predict flow and phase state responses in multi-field coupled numerical models. We developed a multi-field coupled model that considers heat transfer, phase transition, and fluid flow processes to generate high-fidelity data. Additionally, a high-performance surrogate flow model was generated automatically based on the surrogate flow model search (SFMS) approach to significantly reduce time consumption. We conducted comparisons between the surrogate flow model and high-fidelity model for a multi-field coupled process, presenting results for both a single realization and ensemble statistics. The findings show that the proposed surrogate flow model effectively reduces the computational time consumption of multi-field coupled processes and obtains good performance in predicting the flow and phase states. This work is expected to provide ideas for the development of surrogate flow models in the area of complex multi-field coupling.

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Poster / 591

Application of pore throat characteristics research of deep-water globigerina limestones in acid fracturing effectiveness analysis: a case study of the Pearl River Formation in Baiyun Sag, Pearl River Mouth Basin

Authors: Hao Du[1]; Zejun He[None]; Ting Xiong[None]; Jizhi Li[None]; Dongjin Xu[None]; Chenchen Wang[None]; Denglin Han[None]

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Deep-water limestone reservoirs contain a large amount of oil and gas resources. Acid fracturing is an important technical means for the development of carbonate reservoirs, and the compatibility between the acid fracturing method and formation directly determines the development effect of reservoir. A large number of argillaceous and silty globigerina limestones deposited in deep-water

environment on the continental slope are developed in the the Pearl River Formation in Baiyun Sag, Pearl River Mouth Basin. The limestones is composed of micrite, terrigenous debris, and bioclasts, dominated by biogenic cavities, with high porosity and low permeability physical characteristics. Acid fracturing diversion experiments with different acid liquid systems and acid injection methods did not significantly improve the fracture conductivity. Characterize the changes in pore throat structure before and after acid fracturing through casting thin section, micro-CT, electron probes, etc. The experimental results show the bio-cavity backfill corroded seriously with the bio-shell not corroded obviously ; for muddy interstitial materials widely developed in the reservoir, effective dissolution not occurred in acidic environment, exhibited typical high porosity and low permeability to ultra-low permeability characteristics, and the effect of acid fracturing transformation poor (the conductivity under 20MPa is less than 0.005 D·cm); easy to deform (especially under external pressure) due to particle point-contact relationship, argillaceous miscellaneous filled and poor cementation, further blocking the seepage paths. Under the tectonic background, source supply, and sedimentary environment, although carbonate mineral components are enriched, the acid fracturing dissolution effect shows obvious selective characteristics, which improves pore parameters but fails to effectively improve permeability, resulting in poor acid fracturing effect.

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MS15 / **592**

Prediction of Upscaled Permeability of Digital Rock Cores Using Machine Learning Techniques

Authors: Fei Jiang[None]; Lionel Esteban[None]; Mai Shimokawara[None]; Marina Pervukhina[None]; Maxim Lebedev[None]; Mojtaba Seyyedi[None]; Ryuta Kitamura[None]; Takeshi Tsuji[None]; Yaotian Guo[None]; Yoshitake Kato[None]

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A workflow has been proposed to directly predict the upscaled absolute permeability of a rock core from CT images whose resolution is insufficient to directly calculate the pore-scale permeability. The workflow employed the deep learning technique with the raw CT image data of rocks and their corresponding permeability values, which were obtained through high-resolution flow simulation on these images.

A binarized pore-geometry model was first cropped and reconstructed from the high-resolution micro CT images of the rock sample. Then the binarized model was divided into small subsamples of dimensions $100 \times 100 \times 100$, $200 \times 200 \times 200$, and $300 \times 300 \times 300$. To meet the demand of large datasets, the subsamples are allowed to be overlapped during the extraction. The permeability of these subsamples was calculated by the lattice Boltzmann flow solver.

The calculated permeability and corresponding subsample's low-resolution CT image pairs are then input as a dataset to train a neural network (Resnet34). Using the trained Resnet, the permeability map of an extended region in the rock core can be accurately predicted.

Finally, the Darcy flow solver calculates the upscaled absolute permeability of the entire rock core. In this study, we explore the influence of the digital rock subsample core's dimensions and the quantity

of training data on the prediction accuracy and upscaled absolute permeability. Three subsample dimensions, specifically $100 \times 100 \times 100$, $200 \times 200 \times 200$, and $300 \times 300 \times 300$, were evaluated. At a subsample dimension of $100 \times 100 \times 100$, the prediction accuracy was unstable, and good prediction accuracy was not obtained because of the presence of outliers within the subsample where only solid or only void were present. When the subsample dimension was $200 \times 200 \times 200$, the training accuracy was stable and acceptable prediction accuracy was attained when the subsample data size exceeding 20,000. Expanding the sample dimension to $300 \times 300 \times 300$, it was observed that 10,000 training data points were sufficient to achieve satisfactory prediction accuracy.
The findings of our study emphasize that the selection of an appropriate subsample dimension for training data, identified as a Representative Elementary Volume (REV) for upscaling, plays a pivotal role in optimizing the trade-off between computational time and prediction accuracy.

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Poster / 594

Efficient solution strategies for a generalized coupled fluid-porous problem

Author: Linheng Ruan[1]

Co-authors: Iryna Rybak [1]; Paula Strohbeck [1]

[1] *Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*

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Coupled fluid-porous systems appear routinely in environmental, biological, and industrial applications. The flow interaction between the free fluid and the porous medium is strongly interface driven and can be described by the sharp interface or the transition region concept. Classical interface conditions based on the Beavers–Joseph approach are valid only for unidirectional flows parallel or perpendicular to the fluid-porous interface.

In this work, we present a coupling concept which is suitable for arbitrary flow directions. We consider a narrow transition region between two flow domains and derive a hybrid-dimensional Stokes–Brinkman–Darcy model (Ruan & Rybak, FVCA, 2023). The transition zone resolves the storage and transfer of mass, momentum, and energy and can be regarded as a complex interface. We validate the proposed coupling concept numerically against the pore-scale resolved simulations. To solve the coupled problem efficiently, we develop and investigate several preconditioners.

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Ruan, Linheng, and Iryna Rybak. "Stokes–Brinkman–Darcy Models for Coupled Free-Flow and Porous-Medium Systems." International Conference on Finite Volumes for Complex Applications. Cham: Springer Nature Switzerland, 2023.

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MS03 / **597**

Differential Mechanisms of Acidic Fluid-induced Dissolution in Jurassic Ahe Formation Reservoirs across Various Locations within the Northern Structural Zone of the Kuqa Depression

Authors: chaobin Zhu[None]; Denglin Han[None]; Rui Yuan[None]; Hao Du[None]; Kang Yan[None]; Miaomiao Su[None]; Yipeng Li[None]

Corresponding Authors: yuanrui@yangtzeu.edu.cn, zhuchaobin2022@163.com

Abstract: The northern structural zone of the Kuqa Depression exhibits varying lithological characteristics within the Jurassic Ahe Formation, which is predominantly composed of gray to light gray medium-coarse sandstone with high heterogeneity. Based on the structural features of the region, the northern structural zone is divided into the Horst scetion, North slope section, and the Dibei slope section. Among these, the Horst scetion and the Dibei slope section are the main focus of the study. Utilizing techniques such as thin-section observation, scanning electron microscopy, nuclear magnetic resonance, constant rate mercury injection, and micro-CT, the differences in pore structure characteristics of the Ahe Formation reservoir were investigated. This approach aimed to elucidate the causal mechanisms behind the reservoir variations. The Ahe Formation reservoir is primarily composed of lithic sandstone, with dissolution pores being the predominant pore type, followed by micropores. The development of dissolution pores in the Horst scetion is notably superior to that in the Dibei slope section. Additionally, the Horst scetion exhibits larger pore throat radius and better connectivity, leading to a superior pore structure compared to the Dibei slope section. The impact of dissolution processes on pore structure is evident, and therefore, investigating the controlling factors of differential dissolution in various locations within the northern structural zone is crucial for delineating high-quality reservoirs. The Horst scetion represents a Fault~sand transport system, while the Dibei slope section constitutes a Sand~unconformity transport system. Acidic fluids serve as the primary controlling mechanism for the formation of dissolution features in the study area. On a planar scale, dissolution processes are influenced by injection intensity, with greater injection intensity favoring the occurrence of dissolution. Vertically, these processes are governed by conduit systems. In the study area, fluid migration is significantly more pronounced in conduit systems dominated by faults compared to those dominated by sand bodies. The variation in migration patterns at different locations within the northern structural zone results in differing intensities of dissolution processes, leading to variations in pore structure within the Ahe Formation reservoir.
Key word: The Kuqa depression, Dissolution pore, Microscopic pore structure, Accumulation period, Transport system

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MS01 / 598

H2 flow and displacement in sandstone rocks: evaluating experimental results against pore-network model

Author: Zaid Jangda[1]

Co-authors: Tom Bultreys [2]; Zeyun Jiang ; Andreas Busch [1]; Sebastian Geiger ; Kamaljit Singh [1]

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Understanding the pore-scale displacement and trapping mechanisms for hydrogen-brine systems in porous rocks is pivotal as efforts increase to develop subsurface hydrogen storage facilities. Pore-scale flow visualization experiments serve as an important tool to comprehend the pore-scale mechanisms during hydrogen (H2) injection and withdrawal. However, conducting such experiments, particularly under subsurface conditions, are intricate and resource intensive. Quasi-static pore-network models (PNMs) offer a faster alternative to understand multiphase flow in porous media. These simplified models represent pore spaces as networks comprising pores and throats with idealized geometries, simulating fluid invasion based on the quasi-static 'invasion' capillary pressure required for fluid entry. PNMs have been extensively used to simulate multiphase fluid flow behaviour for oil-water systems in porous media, however their utilization for H2-water systems remains limited. In this work, we use a widely used PNM 1 to simulate H2-water flow on two distinct networks, one from a homogeneous rock sample and another from a heterogeneous layered rock sample. We then compare these simulated results with recently conducted pore-scale 3D visualization experiments on both rocks 2, [3]. Comparative analysis indicates a good agreement between PNM simulations and experimental results for drainage and imbibition in the homogeneous case, and reasonable agreement in the heterogeneous case during drainage. However, it is apparent that while PNMs offer a simplified and computationally efficient means to simulate hydrogen flow and displacement in porous media, they cannot presently supplant experimental observations, particularly for complex rocks. This study emphasizes the necessity for further validation of these models against experimental findings to expand their usage and refine simulation predictions.

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MS20 / **599**

Efficient mixed-dimensional models for root water uptake

Author: Timo Koch[1]

[1] *University of Oslo*

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Root water uptake efficiency and robustness to varying soil water distribution depend on the three-dimensional root system architecture.
Roots can also redistribute soil water through the root system. However, roots are numerous and thin which is why modeling root water uptake with three-dimensionally resolved roots is a numerical challenge. Moreover, soil hydraulic conductivity nonlinearly decreases with soil water content resulting in a large conductivity drop in the vicinity of roots which may require local grid refinement around roots to resolve pressure gradients in dry soils.

We first present several approaches to overcome these challenges. We show that a rather coarse-grained approximation of the solution locally around the roots can be combined with local analytical approaches to reconstruct accurate root-soil interface conditions. We discuss the difference between time-independent and time-dependent approximations.
We then demonstrate many challenging numerical tests including a recent benchmark study that compares models from different research groups.
We briefly discuss the implementation of mixed-dimensional schemes in the open-source simulator DuMux.

Finally, we discuss some open questions regarding the inclusion of more complex interface physics in such mixed-dimensional models and detail the challenges stemming from the construction of the interface reconstruction model.

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Poster / 600

Dynamic X-ray computed microtomography imaging of multi-phase flow in porous media using deep learning

Author: Eric Sonny Mathew[1]

Co-authors: Dorthe Wildenschild [2]; Samuel Jackson [3]; Peyman Mostaghimi [4]; Kunning Tang [4]; Ryan Armstrong [4]

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Dynamic imaging of multiphase flow in porous media using X-ray microcomputed tomography (micro-CT) has been a technique exclusive to synchrotron-based systems. With the emergence of deep learning, however, the lower X-ray flux from a standard micro-CT system, and thus lower signal and higher noise under dynamic imaging conditions can be compensated for by use of convolutional neural networks with a *priori* knowledge of the imaged domain and the noise signature.

In this work, a cycle consistent generative adversarial network (CycleGAN) based on the principle of unpaired image-to-image translation is utilized for transforming noisy micro-CT images to clean images. The two main objectives of this study are to assess the levels of noise that would be prevalent during dynamic imaging, and to design a DL network to denoise these images. To obtain the relevant data, fast and slow scans were performed at set saturation levels in the sample. The examined two-phase flow system consisted of air and water (the latter doped with potassium iodide –KI). The sample in consideration was a Bentheimer sandstone sample and the experiment was conducted with a custom-built benchtop micro-CT system located at Oregon State University. To obtain ground truth (GT) images for the training of the CycleGAN model, a high-quality dry scan of the sample was acquired before the KI doped water was injected. Once the fluid was injected, subsequent fast scans were acquired, and finally, a high-quality multiphase scan was captured.

The results from denoising micro-CT scans indicate that the proposed workflow is robust and capable of improving the quality of images with good accuracy and ease of implementation. The fastest scan was conducted at 1min43s while the high-quality scans were acquired at 1hr24mins. Three fast scans with varying scan times of 1min43s, 2min45s, and 3min26s were tested. It was observed that when subjected to the CycleGAN network, the denoised images of 1min43s were adding features (often called hallucinations) in the generated results indicating that the images were too noisy as a starting point. On the other hand, 2min45s and 3min26s scans showed promising results. The accuracy of denoising was then validated by pixel-wise accuracy of the segmented denoised images.

In multiphase flow imaging, it is often not practical to acquire paired images for denoising. With the implementation of cycleGAN, the proposed research not only enhances image quality, but also indicates that the acquisition time can be decreased by more than 25 times from hours to minutes (as low as 2min45s) for dynamic imaging in standard benchtop systems.

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MS06-A / 602

Seepage Model of Conglomerate Based on Deep Neural Network and Finite Element-Discrete Element Coupling

Authors: Kang Yan[1]; Denglin Han[None]; Chenchen Wang[None]; Binyu Ma[None]; Miaomiao Su[None]; Chaobin Zhu[None]

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When previous researchers reconstructed three-dimensional rock models based on two-dimensional images (cast thin sections, electron microscopy, CT slices), they usually modeled based on particle size distribution, replacing particles in the model with spheres. This method is suitable for rocks with good particle size sorting. However, the sorting of conglomerates is poor, the particle size of large particles and small particles differs by several orders of magnitude, which can easily cause large errors in calculations. At the same time, the particle morphology of conglomerates is also complex, and the impact of morphological features on permeability can no longer be ignored.

This paper proposes a method for reconstructing a seepage model based on a deep neural network and Finite Element-Discrete Element Coupling, targeting the influence of particle size distribution and particle morphology in conglomerates on permeability characteristics. The method is divided into three steps: (1) Use a deep neural network to perform semantic segmentation on two-dimensional images, dividing the image into large particle blocks, small particle blocks, and pores; (2) According to the particle size distribution and porosity of the small particle blocks, use the discrete element method for three-dimensional reconstruction, and combine CFD for seepage simulation; (3) According to the morphological features of the large particle blocks, convert them into finite element plane models, and couple them with the discrete element models to calculate the predicted permeability of the original two-dimensional image.

This paper compares the predicted permeability with physical experimental results and the classic Kozeny-Carman prediction equation, verifying the accuracy and superiority of the method in this paper. The main work and conclusions of this paper are: (1) The method in this paper can effectively consider the impact of particle shape on permeability characteristics and improve the prediction accuracy of permeability; (2) The method in this paper can make full use of the information of two-dimensional images, reducing experimental costs and calculation time; (3) The method in this paper has a certain universality and can be extended to other types of porous media.

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MS09 / 604

Simulation of boundaries and parameters variations of natural gas hydrate in thermofluidic dissolution based on multi-field coupling under pore-scale modeling

Authors: Zhengyi Li[1]; Zhiyuan Wang[2]

Co-authors: Chiyu Xie [3]; Hongqing Song [3]; Jianbo Zhang [2]

[1] *China University of Petroleum (East China); University of Science and Technology Beijing*

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When natural gas hydrates are heated and dissolved, the boundaries of fluid-solid will apparently be changed, and average permeability and equivalent thermal conductivity change in coupling. We designed two different microstructures, grain-coating type and pore-filling type, based on two common storage modes. The model size is 50 μm × 22 μm, and the solid particles are 2.0 μm × 2.0 μm. Then we use the Dual Distribution Function model (DDF) of Lattice Boltzmann method to simulate the processes of hydrate dissolution and heat convection based on coupling thermal-flowing-mechanic-chemical (TFMC).

To reduce the impact of nonlinear conditions on calculation results, it is necessary to partition the simulation area along the flowing direction and calculate the data of each partition. The grain-coating type has an initial hydrate saturation of 43.6% and its permeability, as determined by Darcy's law, increases from 0.43D to 2.91D. Similarly, the pore-filling type model has an initial hydrate saturation of 36.6% and its permeability increases from 0.43D to 2.64D. The relationship between permeability K and hydrate saturation Sh is linear, as the simulation area was divided into four equal parts. However, the relationship between thermal conductivity (λ) and hydrate saturation (Sh) in both models is non-linear, which calculated by the convective heat transfer formulation. As the hydrate saturation decreases, the equivalent thermal conductivity firstly increases exponentially and then linearly. The initial thermal conductivity λ of the two models is about 1.47, and the final λ of the grain-coating type is about 8.47, and the final λ of the pore-filling type is about 11.63. Both models split at around 2/3 of initial saturation. The thermal conductivity equivalent, λ, is exponential with saturation from the starting point to the cut-off point, but becomes linear when saturation is less than the cut-off point. The exponential approximation is due to the high proportion of hydrates and the gradual weakening of the thermal diffusion rate compared to the convective heat transfer rate.

To investigate the multi-field coupling effect of TFMC, we analysed the flow rate (seepage field), the initial hydrate saturation Sh (solid field) and the activation energy ΔE or phase change potential ΔH (chemical field). Changes in velocity will not affect the linear relationship of permeability, but will significantly increase thermal conductivity and shorten the nonlinear section. The changes of initial hydrate saturation Sh will not affect the linear law of permeability, but it is necessary to increase the number of calculated partitions to make the results more linear. The demarcation point of equivalent thermal conductivity is kept on about 2/3, only the final results are changed. The activation energy

change (ΔE) and phase change potential (ΔH) indicate different types of hydrates. The permeability or equivalent thermal conductivity do not change significantly.
In summary, the DDF-LBM can be used to simulate the unsteady convective heat transfer process of hydrate dissolution. According the above analysis, more accurate parameters can be provided for thermal flow mining natural gas hydrate under seafloor, which considering the multi-field coupling conditions of TFMC.

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MS06-B / 608

A gel front liquid system with delayed properties for pore-type cracks

Author: Doudou Wang[1]

Co-authors: Yuhuan Bu [1]; Chang Lu [1]; Huajie Liu ; Shenglai Guo [1]

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With the deepening of oil and gas resources exploration and development, drilling wells will encounter various problems, especially the leakage problem, which will lead to a substantial increase in drilling costs. At the same time, the uncertainty of the leakage channel in the process of reservoir leakage not only has a great impact on the drilling efficiency but also causes a large amount of drilling fluid leakage and other problems. At this stage, cement slurry plugging material is the most commonly used plugging material to deal with cracks, holes, and other malignant leakage, but the disadvantage of cement slurry is easy to be dilute with formation water mixing, so it is difficult to stay in the leakage layer in the near-well zone to the point that it can't form a dense blocking layer, so the effect of the cement plugging agent isn't particularly ideal. This paper uses anionic polyacrylamide HPAM and organic chromium crosslinker, a stabilizer to form a temperature and PH-sensitive gel system, the gel system can be added to the pre-positioning liquid to delay the gel formation time, and the system before and after the addition of the pre-positioning liquid, respectively, the performance of the analysis and evaluation, and ultimately determine the gel system. It was found that within a certain range, the release rate of Cr3+ from the organochromium crosslinker in this system accelerated with the increase in temperature, and the release rate of Cr3+ was slower when the pH was 5-7. Since the release rate of Cr3+ determines the speed of hydroxyl bridge reaction with HPAM, the purpose of delayed gel formation in a weak acidic environment can be achieved by controlling these two variables, so that the predisposed liquid system added into the gel can be controlled and sealed after arriving at the target layer, obtaining good plugging effect and laying the foundation for the future cement cementing process.

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MS10 / 610

An AI-based method to measure pores in imaging data with Avizo Software

Author: Eric Pui Lam Ho[1]

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Corresponding Author: eric.ho@thermofisher.com

After imaging samples with CT or FIB-SEM, correctly and precisely detecting pores in the digital acquisition requires image segmentation. A series of steps are necessary to be able to correctly process the data. Firstly, a series of filters must be applied to prepare the data for segmentation. Then a segmentation method must be selected. Finally, each detected pore must be measured.

With the use of AI this process is greatly simplified and datasets where segmentation was previously very challenging can now provide pristine results.

Avizo Software already offered a variety of traditional segmentation tools. With the advent of AI, we now offer the possibility to label, train and execute your AI model in a single application to detect and measure the pores in your material.

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Poster / 611

DuMux – an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling

Authors: Timo Koch[1]; Dennis Gläser[2]; Martin Schneider[2]; Bernd Flemisch[2]

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DuMux (https://dumux.org/) is a general simulation framework (written in C++) with a focus on finite volume discretization methods, model coupling for multi-physics applications, and flow and transport applications in porous media. Its core applications are single and multiphase flow applications in porous media on the Darcy scale, embedded network and fracture models, and free-flow porous media flow interaction. However, it can also be used as a general-purpose finite volume / control-volume finite element solver for partial differential equations. Pre-implemented models, make it a versatile tool for many porous media applications.

In this poster contribution, we give a brief overview of the main features and application areas. Moreover, we present updates in recent years (including the upcoming release of DuMux version 3.9, Spring 2024) and how the capabilities have improved since the initial appearance of DuMux 3.0 (which is described in 1). Novelties include additional (pore-)network modeling capabilities, 2D shallow water equations (e.g. for river modeling), new control-volume finite element schemes, methods for free-flow porous media coupling, fractured porous media, multithreaded assembly, and new tutorials and educational material.
Given the theme of the conference, we put a special emphasis on “Porous Media & Biology” applications and models in DuMux.

DuMux is based on the DUNE framework from which it uses the versatile grid interface, vector and matrix types, geometry and local basis functions, and linear solvers. DuMux then provides finite volume discretizations (Tpfa, Mpfa, Staggered) and control-volume finite element discretization schemes (P1, CR/RT, MINI); a flexible system matrix assembler and approximation of the Jacobian matrix by numeric differentiation; a customizable Newton method implementation, and many pre-implemented models (Darcy-scale porous media flow, Navier-Stokes, Geomechanics, Pore network models, Shallow water equations) and constitutive models. DuMux features a multi-domain framework for model coupling suited to couple subproblems with different discretizations/domains/physics/dimensions/… and create monolithic solvers.

Acknowledgement: DuMux has been developed since 2010 with contributions from over 80 developers. The poster contribution will mention the poster authors and acknowledge an updated list of developers actively contributing to DuMux since the release of version 3.0.

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1 https://doi.org/10.1016/j.camwa.2020.02.012

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Poster / 612

Time-dependent deformation of porous sandstones during pore pressure fluctuations and its effect on porous sandstone properties: Implications for subsurface hydrogen storage.

Author: Ming Wen[1]

Co-authors: Nick Harpers [1]; Jim Buckman [1]; Kamaljit Singh [1]; Andreas Busch [1]

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In underground hydrogen storage operations, reservoir rocks often experience periodic pore pressure fluctuations due to annual or more frequent gas extraction and injection cycles. These fluctuations subject the reservoir rocks to cyclic effective stress changes, causing their mechanical and transport behaviours to differ from those under static conditions. However, understanding how porous rocks react to pore pressure oscillations in situ conditions is still limited. To address this, we selected three types of sandstones with different physical properties (Castlegate, St Bees, and Zigong sandstone, respectively), and conducted pore pressure oscillation experiments over several weeks at different rates and amplitudes to simulate underground hydrogen injection and extraction processes. Permeability was periodically measured during the initial loading phase and stress cycle intervals. 3D images of the samples before and after pore pressure cycling were obtained by performing X-ray micro-computed tomography scans, and digital core models were established to characterise the geometric topological features of the three sandstones quantitatively. Experimental results indicate that all three types of sandstone exhibit more significant increases in axial strain and decreases in permeability than the control groups under constant pore pressure conditions. The strain changes induced by these stress cycles were the primary control on permeability decline in the sandstones. Notably, in the case of the high-porosity Castlegate and St Bees sandstones with porosities of 19.8% and 18.6%, respectively, we observed that both the accumulation of inelastic strain and the decrease in permeability were positively correlated with an increase in the rate, amplitude, and cycles of pore pressure oscillations. In contrast, for the Zigong sandstone, which has lower porosity, there was no obvious correlation among these factors. Microstructural evidence based on CT analysis revealed that the inelastic deformation mechanisms in the three types of sandstones were dominated by grain rotations and rearrangements. However, compared to Zigong sandstone, characterised by its closely packed grains and lower porosity, only 7.9%, Castlegate and St Bees sandstones demonstrated more pronounced changes in pore structure and a more significant loss in porosity. This implies that sandstones with higher porosity, having more space to accommodate grain movements and rearrangements, are more sensitive to rapid pressure changes during cyclic loadings, leading to a more significant response of their physical properties to pore pressure cycling.

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Poster / 616

Visualized investigation of transport behaviors during CO2-EOR in multiscale porous medium

Author: Jiawei Shi[1]

Co-authors: Linyang Tao [2]; Bo Bao [3]; Junjie Zhong ; Liyuan Zhang [1]

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Although CO2 injection into the geological formations is a promising option to enhance oil recovery, how multiscale pore structures within porous media affects multiphase transport remains poorly understood. This study fully exploits the unique advantages of real-time in-situ visualization of microfluidics to investigate the multiphase flow behavior within micro and nano-pores during both CO2 miscible and immiscible flooding process. Two types of porous media chips with network channel structures were designed–a micro-nano scale cross-scale chip with a fracture-matrix structure and a micro-scale chip with multiple pore-throat ratios. This study investigates the impact of cross-scale effects, Jamin effect, and network channel shapes on the flow patterns of CO2 and oil during the CO2 flooding process. The effects of these factors on the recovery rates throughout the entire CO2 flooding process are also discussed. In the cross-scale chip, micro-scale fracture channels expedite the process of achieving a 100% recovery rate in CO2 miscible flooding. Conversely, the micro-scale fracture channel, offering a "short circuit" pathway for CO2, results in the extensive entrapment of residual oil, leading to a substantial reduction in the recovery rate in CO2 immiscible flooding. In the micro-scale chip, the flow resistance induced by the Jamin effect increases with the increase of the pore-throat ratio porous media during CO2 immiscible flooding. The time required to achieve 100% recovery efficiency during CO2 miscible flooding is notably delayed with an increase in the pore-throat ratio. These results can significantly enhance our understanding of multiphase transport in CO2 enhanced oil recovery, facilitating the optimization of practical CO2-EOR schemes.

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MS18 / 617

Conducting Monitored Natural Attenuation: Microbial communities hold the answers

Authors: Lu Yang[None]; Shaopo Deng[1]

Co-authors: Qiang Chen [1]; Jing Wei [1]; Tingting Fan [1]; Lingya Kong [1]; Tao Long [1]; Shengtian Zhang [1]

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The application of Monitored Natural Attenuation (MNA) technology has been widespread, while there is a paucity of data on groundwater with multiple co-contaminants. This study selected a high permeability and low hydraulic gradient with BTEX (benzene, toluene, ethylbenzene, and xylenes), chlorinated aliphatic hydrocarbons (CAHs) and chlorinated aromatic hydrocarbons (CPs) co-contamination to unravel the responses of microbial communities during natural attenuation processes. The results showed that the diversity and composition of groundwater microbial community exhibited greater variation horizontally than vertically. Groundwater microbial community was primarily shaped by the total quantity of contaminant ($r = 0.722$, $p < 0.001$), and BTEX would have a more significant influence on community diversity than CAHs or CPs especially at high zone. The groundwater microbial community assembly was governed more by deterministic processes ($\beta NTI < -2$) than by stochastic processes in high contaminants concentration zone and showed an opposite trend at low-concentration zone ($|\beta NTI| < 2$). The co-occurrence relationships among microorganisms indicated that the differences in degradation mechanisms at various depths. This study provided a better ecological understanding for preparation of long-term monitoring plan at further MNA practices of deep thick and multiple co-contaminants aquifers.

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618

Bio-reactive Transport Modeling in Underground Hydrogen Storage: Current Status, Challenges, and Perspectives

Authors: Gloire Imani[1]; Hai Sun[2]; Lei Zhang[None]

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In the wake of escalating concerns about climate change and the looming specter of the greenhouse effect, governments worldwide have embarked on ambitious initiatives to mitigate carbon emissions and transition towards sustainable energy solutions. As carbon-intensive energy sources continue to contribute to the greenhouse effect, the imperative to harness cleaner alternatives has never been more urgent. Amidst this backdrop, the focus on hydrogen—a versatile and environmentally friendly energy carrier—has intensified. The storage of hydrogen underground presents a compelling solution for large-scale, long-term storage. However, the underground surfaces earmarked for hydrogen storage are not mere geological repositories; they are bustling ecosystems teeming with microbial life. Whether in the porous rock formations of depleted reservoirs, the expansive voids of salt caverns, or the porous structures of aquifers, microbes interact with hydrogen and lead to hydrogen consumption. This intricate dance between hydrogen, geological formations, and microbial communities lays the foundation for the emergence of bio-reactive transport modeling. However, bio-reactive transport in porous media involves scales ranging from the bacteria scale to the aquifer heterogeneity scale and a temporal multiscale nature of the various phenomena involved, such as flow, transport, and biofilm growth. Thus, the existing bio-reactive models have several limitations in UHS. Furthermore, the effects of microbes on pore-scale phenomena such as wettability alteration have not been modeled yet. The impacts of microbial activities on macroscale properties, including capillary pressure and relative permeability, have not yet been understood. The development of visualization techniques (micro-CT) capable of capturing microbial activities in real rock would significantly help in constructing accurate bio-reactive models.

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MS06-A / 619

Interpreting Pore-Scale Fluctuations: Predicting Transport Coefficients in Multiphase Flow through Porous Media Using the Green Kubo Formulation - An Experimental Investigation

Author: Umar Alfazazi[1]

Co-authors: DIck Bedeaux [2]; Signe Kjelstrup [2]; Marcel Moura [3]; Mohammad Ebadi [4]; Peyman Mostaghimi [1]; James McClure [5]; Ryan T. Armstrong [1]

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Pore scale fluctuations during multiphase flow in porous media have been observed over the past decade particularly at capillary dominated flow regimes. While multiphase flow in porous media is typically predicted using models that employ average properties, the current models do not incorporate these fluctuations at the pore scale. It therefore remains unclear how flow fluctuations can be integrated into existing models and to what degree they are related to energy dissipation.
Herein, we study pore scale fluctuations during steady state multiphase flow using the concept of non-equilibrium thermodynamic and statistical mechanics. We investigate, for the first time, how the Green Kubo formulation of the fluctuation dissipation theorem (FDT) can be used to predict the transport coefficient from the two-phase extension of Darcy's law. Flowrate-time series data are recorded at the millisecond time scale using a novel experimental setup that allows for the determination of flow fluctuation statistics. Steady state coreflooding experiments were conducted using DI water and decane as the wetting and non-wetting phase. A water fractional flow of ~0.5 was used while varying the total capillary number, Ca. By using Green Kubo relations, a transport coefficient is predicted based on the integrated autocorrelation function (ACF). The transport coefficient using conventional Darcy's linear law was also compared with the FDT approach.
Notable fluctuations were observed at all Ca studied. A linear relationship between average flux and pressure drops was observed at the lowest Ca. Hence, obeying Darcy's law. At higher Ca but still within capillary dominated flow regime, there was a systematic deviation from the linear trend. Thus, a non-Darcy behaviour was observed. Statistical frequency analysis of the flow fluctuations further shows non-Gaussian feature, that is more pronounced at the lowest Ca. By using Green Kubo relations, a transport coefficient is predicted based on the integrated ACF. Notably, this coefficient aligned closely with the total effective phase mobility computed using Darcy's equation for multiphase flow, particularly in scenarios where a linear relationship between flow rate and pressure gradient was observed. We provide the first experimental evidence of using FDT to determine transport coefficient during multiphase flow in porous media.
Our results open a new application for nonequilibrium thermodynamics where microscale fluctuations during multiphase flow are directly linked to macroscale parameters. Establishing a connection between these fluctuations and macroscale parameters is pivotal to understanding energy dissipation during multiphase flow and associated modes of transport.

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Poster / 620

The Wettability Evolution Process and Mechanism of Deep Tight

Sandstones Controlled by Diagenesis: A Case Study from the Dongying Sag, Bohai Bay Basin

Author: Xin Wang[None]

Co-author: Jianhui Zeng [1]

[1] *China University of Petroleum, Beijing*

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Abstract: Wettability plays a crucial role in the percolation capacity of deep tight sandstone reservoirs. Due to great variations in fluid properties, mineral types, and compositions during diagenetic evolution processes, the wettability evolution process and its control mechanism remain unclear, which limits the understanding of hydrocarbon accumulation in deep tight sandstones. In the present study, the upper submember of the 4th member of Shahejie Formation in Dongying Sag, Bohai Bay Basin is targeted to systematically analyze the influence of diagenesis on deep tight sandstone reservoir wettability. A combined method including cast thin sections, X-ray diffractions, high-temperature and high-pressure Amott wettability experiments attached to a nuclear magnetic resonance equipment, and high-temperature and high-pressure solid-oil-water contact angle experiments. The results show that the different types of pores have been generated in different diagenetic stages. From A-stage eodiagenesis to B-stage mesodiagenesis, the compaction residual pores, dissolution pores in feldspar and dissolution pores of carbonate, dissolution pores of quartz margin, dissolution pores in feldspar and dissolution pores of carbonate, fractures wee formed in sequence. With the ongoing diagenesis, the water wetability of residual intergranular pores, the dissolution pores of quartz margin and the dissolution pores in feldspar are enhanced, while the dissolution pores of calcite become more oil wetting, and the dissolution pores of dolomite change from water wetting to intermediate wetting. In addition, the main pore types developed at different diagenetic stages and their surface wetting characteristics determine the overall wettability of deep tight sandstone. Overall, the deep tight sandstone is mainly characterized by water ettability, which is changed from strong water wetting, weak water wetting, water wetting, intermediate wetting, to water wetting from A-stage eodiagenesis to B-stage mesodiagenesis. A wettability evolution model for deep tight sandstone reservoirs controlled by diagenesis is established, which holds significant implications for predicting sweet spots in deep tight sandstone reservoirs.
Key words: Jiyang Depression; Beach-bar Sand; Deep Reservoirs; Diagenesis; Magnetic Resonance Imaging

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MS10 / 623

Spectral micro-CT imaging of soil: retrieving atomic information and density maps

Author: Marijn Boone[1]

Co-authors: Bert Masschaele [1]; Denis Van Loo [1]; Jan Dewanckele [1]; Wesley De Boever [1]

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Introduction

Micro-CT is a unique technology to non-destructively investigate the internal structure of samples, spanning a range from centimeter to micrometer scale. However, when it comes to material identification, the technology has some inherent limitations. The contrast observed within a micro-CT scan arises from a multitude of factors. The attenuation coefficient of a material is influenced not only by its atomic number and density but also by additional variables such as X-ray energy, the X-ray spectrum, and the characteristics of the employed detector. These diverse factors collectively contribute to the observed contrast, making the process of material identification in micro-CT scans a nuanced and multifaceted endeavor.
By using a spectral detector, not only the attenuated intensity of the X-ray beam can be measured, but the energy spectrum of the X-ray beam is captured when it passes through a sample. This capability facilitates the segregation of information relating to both the atomic number and density within the spectral scan.

Materials and Methods

A contaminated soil sample was into a 7 cm diameter container and scanned on a TESCAN UniTOM XL SPECTRAL using both traditional attenuation-based tomography and spectral tomography which allows to measure the entire energy spectrum between 20 and 160 keV of the X-ray beam. The spectral data was reconstructed and analyzed using the TESCAN Spectral suite, which enabled to extract spectra and analyze K-edge information from dense mineral phases in the sample and generate maps of the atomic information (Zeff) and the density in the soil.

Results and Conclusion

In this work we show how spectral micro-CT can improve material identification for porous geological material like soil. The soil was contaminated with heavy metals and the spectral K-edge imaging was used to analyze the distribution lead in the soil. This is illustrated in figure 1, where the spectral signature of 2 dense grains is shown. The presence of the K-edge of Pb in one of the spectra is clearly present, positively identifying lead bearing particles in the soil.
The attenuation coefficient in a micro-CT image depends on the X-ray energy, the atomic number and the density. Because we have information of all the X-ray energies between 20 and 160 keV in the spectral CT a better distinction between the atomic information (Zeff) and density can be made. In the soil we have larger granules in a finer grained matrix. In figure 2 we can see that in the Zeff map there is no difference between the granules and the matrix. While in the density map the matrix and granules can clearly be discriminated. This shows that the granules in the soil have the same chemical composition as the matrix (same Zeff) but have a clear difference in density, where the granules are far denser compared to the matrix.
All results show the large potential of spectral CT in enhancing attenuation-based micro-CT and providing new and unique insights in all types of materials.

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Single well system rectangular reservoir pressure buildup

Author: Qing Nie[None]

Co-authors: Jing Lu ; Erlong Yang

Corresponding Author: 871789003@qq.com

In this paper, a new mathematical model of pressure buildup in a closed rectangular reservoir under constant bottom-hole pressure and constant production is presented. The model is designed to provide approximate analytical solutions to pressure variations in rectangular reservoirs in order to gain a deeper understanding of reservoir productivity and production behavior. Compared with the empirical or semi-analytical models in the literature, the model proposed in this paper is completely analytical and has a solid theoretical basis, which can accurately predict the production performance of a single well under constant bottom-hole pressure. The model is obtained by a series of mathematical methods such as Laplace transform, Dirac function, convolution, Green function and superposition principle. The effects of reservoir area, well location, shut-in pressure and production time on shut-in pressure buildup in closed rectangular reservoirs are analyzed. This paper provides a powerful tool for the field of oil and gas engineering to better plan and manage reservoir development.

Key words: Rectangular reservoir; Pressure buildup; Mathematical model

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MS17 / 628

Investigating the effects of temperature and moisture on CH4 recovery after CO2 injection: flow simulation based on coal pore network model

Author: Qiaoyun Cheng[1]

Co-authors: Sandong Zhou (Corresponding Author) [1]; Zhejun Pan [2]; Dameng Liu [3]; Detian Yan [4]

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The massive burning of fossil fuels has led to a dramatic increase in the level of CO2 in the atmosphere, which has greatly affected the global ecology and climate. CO2 enhanced coalbed methane recovery technology not only reduces the CO2 footprint in the atmosphere, but also effectively promotes the extraction of CBM. Coal has strong heterogeneity and dual pore structure, and after CO2 is injected into the coal reservoir, a complex binary gases (CO2 and CH4) flow and multi-physical field coupling problems will occur. we are still confronting of tricky challenges in study the flow of binary gases under multi-field coupling conditions in complex pore networks.

In order to truly restore the pore structure of coal and the flow characteristics of binary gas, this work conducted X-ray scanning on coal samples collected in South Junggar, China, and 3D reconstructed the coal samples using the obtained two-dimensional CT slices. Based on the reconstructed pore network model, permeability simulation was performed using the finite element method. Penetration and diffusion of binary gases and water as well as heat and mass transfer are considered during the simulation. This study aims to investigate: (1) The main factors controlling the competitive adsorption/desorption capabilities of binary gases. By comparing the simulation results of different CO2 injection pressures, reservoir temperatures and moisture content, to clarify the main factors affecting the competitive adsorption capacity of CO2 and CH4. (2) Reservoir temperature changes induced by binary gas adsorption/desorption. Gas adsorption is an exothermic reaction, and the desorption is an endothermic reaction. Due to the adsorption/ desorption dynamic changes of dual gases in the system, the temperature of the reservoir has a periodic law. (3) Permeability evolution rules of binary gases and recovery efficiency of CH4. Reservoir temperature and water content in pore network have a great impact on gas production efficiency. By ignoring and considering two factors during the simulation process, to determine the impact on the permeability change of the binary gas and the recovery efficiency of CH4.

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(1) Fan, YP, Deng, CB, Zhang, X, et al. Numerical study of CO2-enhanced coalbed methane recovery. International Journal of Greenhouse Gas Control. 2018, 76: 12-23. (2) Merkel, A., Gensterblum, Y., Krooss, BM., et al. Competitive sorption of CH4, CO2 and H2O on natural coals of different rank. International Journal of Coal Geology. 2015, 150: 181-192. (3) Liu, SQ., Fang, HH., Sang, SX., et al. CO2 injectability and CH4 recovery of the engineering test in qinshui Basin, China based on numerical simulation. International Journal of Greenhouse Gas Control. 2020, 95: 102980. (4) Fang H.H., Sang, S.X., Wang, Z.F., et al. Numerical analysis of temperature effect on CO2 storage capacity and CH4 production capacity during the CO2-ECBM process. Energy. 2024. doi: https://doi.org/10.1016/j.energy.2023.130022. (5)

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Poster / 630

Pore-Scale Exploration of Wettability Impact on Fluid Flow: Micro-CT Imaging and Relative Permeability Analysis in a Sandstone Core

Author: Tingting Wang[None]

Co-authors: Kunning Tang [1]; Peyman Mostaghimi ; Ryan Armstrong ; Ying Da Wang [1]

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In recent years, advancements in micro-computed tomography (micro-CT) imaging technology and image processing have significantly enhanced our understanding of the internal structure of rock cores and the distribution of fluids during multiphase flow. Herein, we utilize micro-CT to explore the impact of wettability on fluid flow in a sandstone rock at the pore-scale in combination with relative permeability measurements by history matching steady state flow experiments. Steady state experiments were conducted by the co-injection of decane and water into a sandstone core under different fractional flows (Fw=0, 0.25, 0.5, 0.75, and 1) and wetting conditions. At each stabilized fractional flow, the system was imaged with micro-CT at a resolution of 6.7μm under dynamic flow conditions. The sandstone core as initially tested in a clean state, i.e., water-wet condition, followed by aging in crude oil for two weeks at 90oC to create an aged state core, i.e., oil-wet/mixed-wet condition. For the aged-state core, it was observed that the oil-water interface was dynamically changing under so-called steady state conditions while the clean state core provided static connected pathways for flow. Consequently, the aged-state core was also imaged under static conditions to capture fluid/fluid interfaces and common lines. Based on the scanned images, parameters such as contact angle, curvature, pore occupancy, and Euler number were calculated, comparing differences between the clean state and aged-state conditions. Furthermore, history matching of relative permeability was performed to analyse the flow characteristics at the continuum scale, providing a comprehensive understanding of pore-scale mechanisms linked to relative permeability behaviour.

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MS15 / 631

A Transformer-based framework for brine-gas interfacial tension prediction: Implications for H2, CH4 and CO2 geo-storage

Author: Tianru Song[1]

Co-authors: Ming Yue [1]; Hussein Hoteit [2]; Hassan Mahani [3]; Stefan Iglauer [4]; Bin Pan [1]

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Brine-gas interfacial tension (γ) is an essential parameter to determine fluid dynamics, trapping and distributions at pore-scale, thus influencing gas storage capacities and securities at reservoir-scale. However, γ is a complex function of pressure, temperature, ionic strength and gas composition, thus very time-consuming and costly to cover all these influencing factors by experiment. Therefore herein, a machine learning workflow is established to predict γ accurately and and develop a mathematical prediction model under various gas (H2, CH4 and CO2) geo-storage scenarios.
First, three types of gases (namely H2, CH4 and CO2) were encoded based on their molecular weight. Then, γ and its influencing factors were input into the dataset (total 300 data points were collected, and the ratio of the training to the testing dataset is 8 : 2). Next, the advanced Transformer model was used to predict γ with the determination coefficient (R2) to evaluate the prediction accuracy. Finally, an accurate γ prediction correlation is derived as a function of pressure, temperature, ionic strength and gas composition.
The prediction results have shown that:
1) The prediction precision is high with (R2>0.8);
2) under typical gas geo-storage conditions, γ magnitudes follow the order H2 > CH4 > CO2, e.g., γ is 68 mN/m, 62 mN/m, and 27 mN/m respectively at 10 MPa and 50 °C for these three gases;
3) For a representative H2 geo-storage scenario with CO2 as cushion gas, γ for the H2 and CO2 mixture is smaller than that for H2, while larger than that for CO2, which is attributed to various intermolecular forces for various gas compositions;
4) γ decreases with increasing pressure and temperature, while γ does not have a monotonous relationship with I, quantitatively consistent with experimental observations.
To our best knowledge, this is the first time to introduce a robust Transformer-based formula generation framework and develop a mathematical model for cost-effective prediction of γ under a wide range of gas geo-storage conditions. These insights will promote energy transition, balance energy supply –demand and reduce carbon emissions.

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MS03 / 632

Interaction forces caused by relative movement in a continuum mechanical model for suffusion

Authors: Solveig Buscher[1]; Eugen Perau[1]

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Dam failures and landslides can be caused by erosional processes. Suffusion, a special type of internal erosion (Yang et al., 2019), is the initial stage of a backward erosion process (van Beek, 2015) which may lead to creeping degradation of the dam's stability and in the end to catastrophic outcomes like the Brumadinho tailings dam collapse in Brazil 2019 (Silva Rotta et al., 2020). Currently, there are no field-scale models that can predict the time scale of the process and the area of collapse. Only empirical criteria (Chang et al., 2013) can be used to determine whether a soil is erosionally stable or unstable (Fell et al., 2015). New projects could be planned following these criteria. However, some existing earthworks may not meet these criteria and a reliable risk evaluation is not possible. Moreover, for economic reasons, modelling the whole process and, in consequence, predicting the duration of erosion processes may lead to more cost-effective constructions.
To model suffusion at the field scale, the authors are currently researching a continuum mechanical approach. The total soil is modelled with three phases: grain skeleton, water and particles which can be eroded or deposited. These three phases can move independently, and their motion is described by balance equations and constitutive laws. Analog to the effects of suffusion, these laws include the weakening of the soil mechanically. The detachment of particles increases water conductivity, while particle agglomerations impede flow in certain areas, resulting in an increase of seepage forces on the grain skeleton. In a further development of existing approaches by Vardoulakis (2004), the particle diameter is introduced as a parameter. If the particles are very fine and their volume fraction is relatively small, their movement is dominated by advective transport. Consequently, the particles move simultaneously with the water phase. If the particle size is above a certain diameter, friction between particles and water becomes dominant and causes relative motion between these constituents. Additionally, the interaction between the particles and the pore channel of the grain skeleton arises significantly. (e.g., Bear et al., 1987; Schaufler et al., 2012)
A new model based on the Theory of Porous Media (TPM) (Bowen, 1976) represents the mechanical aspects of particle transport through the pore space. Resistivities are defined to represent the interaction forces between the three soil constituents. Observing a special case, the interaction between the soil skeleton and the pore fluid represents the Darcy velocity. The drag force caused by the interaction between particles and pore fluid is also known, but it is typically used for sedimentation and not in combination with the Darcy equation. Additionally, there is an interaction between the particles and the soil skeleton, which has not yet been applied to continuum mechanical models.
Analytical and numerical findings show that the movement of the fluid and particle phases within the pore space can be represented in a continuum mechanical model. The results are plausible for both laminar and non-laminar flow, as well as for different particle concentrations.

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Poster / 633

Study on the Distribution Patterns and Resistivity Characteristics of THF Hydrates in Sandstone Sediments

Authors: Zizeng Li[1]; Qin Dai[1]; Chenyu Li[1]; Ming Chen[2]; Min Li[1]; Fei Xian[1]; Jiamin Hu[1]; Xuefeng Liu[1]

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Investigating the distribution patterns of hydrates in the pore spaces of sedimentary rocks and their resistivity characteristics is crucial for understanding and predicting the storage and extraction of natural gas hydrates. However, CT and resistivity joint measurements indicate that while the distribution of Tetrahydrofuran (THF) hydrates in sandstone sediments is similar to that in conventional oil and gas reservoirs, the resistivity measurements do not fully conform to the Archie model. This discrepancy arises because the formation of THF hydrates is a dynamic process which involves fluctuations in hydrate saturation, formation water salinity, temperature, and spatial distribution, making it challenging to accurately characterize these variables using traditional resistivity measurements. To address this issue and gain a deeper understanding of the complex petrophysical relationships in THF hydrate sediments, this study established digital rock based on the hydrate distribution from in-situ CT scans by segmenting the three-dimensional grayscale images of the sediments. The spatial distribution of hydrates within the sediment pores was then simulated using the Diffusion-Limited Cluster Aggregation (DLCA) model. Subsequently, the resistivity of sediments at various hydrate saturations is determined using the finite element method. The results show that at low hydrate saturations, hydrates exist in a dispersed form within the pores, while at high saturations, they are distributed in cementing or encapsulating forms, enhancing the structural integrity of the sediments. Furthermore, analysis of the aggregate morphology, including changes in gyration radius and fractal dimension, effectively reflects the evolution of the structure. The combined results from experimentation and simulation demonstrate that varying hydrate saturations significantly influence the distribution forms and their impact on resistivity: at low saturations, hydrates have a minor effect on resistivity, whereas at high saturations, extensive hydrate formation and distribution patterns

lead to a rapid increase in resistivity. Overall, this study offers novel insights and methodologies for understanding the petrophysical characteristics.

Keywords：THF hydrate formation, Resistivity measurements, Digital rock, DLCA model, Finite element method.

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MS05 / 637

Field-scale mathematical modelling and simulations of biofilm effects in hydrogen storage

Author: David Landa-Marbán[1]

Co-authors: Svenn Tveit [1]; Tor Harald Sandve [1]; Sarah Gasda [1]

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Underground hydrogen storage (UHS) allows for large-scale energy retention using depleted hydrocarbon reservoirs, saline aquifers, and salt caverns. Biofilms, defined as an aggregate of microbes enclosed in a matrix of extracellular polymeric substance (EPS), are sophisticated systems where different biological, chemical, and physical processes occurs such as growth, erosion, sloughing, attachment, formation of metabolites, etc. While in some applications we can benefit from biofilms (e.g., food industry, water quality), biofilms can also become an obstacle, especially for UHS regarding injectivity and hydrogen loss. Numerical simulations can assist on a better understanding of the interactions between biofilms and hydrogen in cyclic operations involving injection, storage, and withdrawal periods.

The aim of this work is to develop and implement a mathematical model to perform field-scale UHS simulations including biofilm processes. We can find in literature comprehensive multi-component bio-reactive models for UHS (e.g., Hagemann et al. (2016)). Since field-scale simulations require running the model on large spatial and temporal scales, then simplified models are suitable to deal with the heavy computational burden. Still, the simplified model must capture the key processes and quantities. Here, the main mechanisms related to microbial activity are the consumption of hydrogen by the biofilm, porosity reduction due to the development of the biofilm, and biofilm detachment because of higher flow velocities. To this end, the fluid is modelled as a two-phase (liquid and gas), two-component (water and hydrogen) system, while the biofilm is modelled as a solid phase attached to the rock, which grows due to hydrogen consumption and suffers erosion due to the flow.

The mathematical model is implemented in the industry-standard simulator Open Porous Media (OPM) Flow (Rasmussen et al., 2019). The existing hydrogen module implementation is extended to include biofilms, which allows for flexibility to account or neglect the biofilm effects on the simulations. For example, in Strobel et al. (2019) the authors presented a history matching study where microbial activity was identified in the field during hydrogen injection, leading to a successful match after adjusting the initial biofilm density.

We apply the model to assess the hydrogen loss under different injection strategies and microbial parameters. The complexity in the geological models is increased from core samples to layered heterogeneous field-scale reservoirs. We use the pyopmnearwell software (Landa-Marbán and von Schultzendorff, 2023), an open-source framework for creating the required input files by OPM (e.g., corner-point grids, tables for the saturation functions, injection schedules) via configuration files, to perform the simulations, which allows for reproducibility of the results and further studies (e.g., history matching, optimization).

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Poster / 639

A novel CO2-responsive microgel for in-depth conformance control in CO2 enhance oil recovery (EOR)

Author: Qihui Wu[None]

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CO2-EOR (enhanced oil recovery) represents one of the most cost-effective methods for achieving carbon neutrality. However, CO2 flooding encounters serious preferential flow in porous mediums, which significantly reduce the economic benefits of CO2-EOR and exacerbate the risk of CO2 leakage. This study synthesized a tertiary amine-based, CO2-responsive microgel. The microgel possesses a particle size of ~7.50μm in neutral formation water and expands to 2-4 times upon contact with

CO2, thereby offering advantages in deep profile modification and selective CO2 plugging. Core flooding experiments confirmed the microgel's effectiveness in deep profile modification and EOR in heterogeneous reservoirs.

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Poster / 641

Transport and Detachment Characterization of Nanoparticle-Laden Oil Droplet in Pore-Throat Channel

Author: Yue Li[None]

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To enhance the applications of nanoparticles (NPs) in enhancing oil recovery, a crucial aspect is gaining a comprehensive understanding of the transport and detachment mechanisms of oil droplets through a pore throat. A novel, hybrid pore-scale simulation method is proposed, utilizing a combination of Lattice-Boltzmann (LB) and Langevin-Dynamics (LD) approaches to investigate the transport and detachment mechanisms of a nanoparticle-laden oil droplet. The LD method is specifically developed to capture the intricacies of Brownian motion, thermal fluctuation-dissipation, multi-body hydrodynamics, and particle-particle interactions. The discrete LB forcing source distribution is integrated with LD, enabling a comprehensive evaluation of random forces, friction forces, van der Waals forces, and electrostatic forces involved in the transport and detachment of nanoparticle-laden oil droplet in a narrow microchannel. The variation in pressure difference is observed when the oil droplet transport in a narrow channel. And the nanoparticle-laden oil droplet when transporting in the channel shows a less pressure difference compared with oil droplet without NPs adsorbed on. Moreover, with some NPs attached on the channel, there is little oil trapped on the channel. The oil droplet detaches from the channel with the help of NPs. Results demonstrate that oil droplet detachment from a surface is not related with surface wettability and the adsorbed area of NPs is critical in detachment process. The outcomes of this work provide valuable insight into the critical importance of nanoparticles effects on the detachment and transport of oil droplet in porous media.

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MS13 / 643

Confinement-guided self-assembly of ionic superdiscs

Author: Zhuoqing Li[None]

Co-authors: Aileen Raab ; Mohanmed Kolmangadi ; Mark Busch ; Macro Grunwald ; Felix Demel ; Andriy Kityk ; Andreas Schönhals ; Sabine Laschat ; Patrick Huber [1]

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Discotic ionic liquid crystals (DILCs) consist of self-assembled superdiscs of cations and anions that spontaneously stack in linear columns with high one-dimensional ionic and electronic charge mobility, making them prominent model systems for functional soft matter. Compared to classical non-ionic discotic liquid crystals (DLCs), many novel liquid crystalline structures with a unique combination of electronic and ionic conductivity have been reported, which are of interest for separation membranes, artificial ion/proton conducting membranes and optoelectronics. Unfortunately, a homogeneous alignment of the DILCs on the macroscale is often not achievable, which significantly limits the applicability of DILCs. Infiltration into nanoporous solid scaffolds can overcome this drawback. However, little is nknown about the structures of DILCs in nanoscale confinement. Here, we present temperature-dependent high-resolution optical birefringence measurement and 3D reciprocal space mapping based on synchrotron-based X-ray scattering to investigate the thermotropic phase behavior of dopamine-based ionic liquid crystals confined in cylindrical channels of 180 nm diameter in macroscopic anodic aluminum oxide (AAO) membranes. As a function of the membranes hydrophilicity and thus the molecular anchoring to the pore walls (edge-on or face-on) and the variation of the hydrophilic-hydrophobic balance between the aromatic cores and the alkyl side chain motifs of the superdiscs, we find a particularly rich phase behavior, which is not present in the bulk state. It is governed by a complex interplay of liquid crystalline elastic energies (bending and splay deformations), polar interactions and pure geometric confinement, and includes textural transitions between radial and axial alignment of the columns with respect to the long nanochannel axis. Furthermore, confinement-induced continuous order formation is observed in contrast to discontinuous first-order phase transitions, which can be quantitatively described by Landau-de Gennes free energy models for liquid crystalline order transitions in confinement. Our observations suggest that the infiltration of DILCs into nanoporous solids allows tailoring their nanoscale texture and thus their electrical and optical functionalities over an even wider range than in the bulk state, in a homogeneous manner on the centimeter scale as controlled by the monolithic nanoporous scaffolds.

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MS18 / 644

A trend prediction model of natural attenuation in groundwater based on machine learning and microbial community

Authors: Xiaodong Zhang[1]; Ran Yu[2]; Tao Long[1]; Xin Zhu[1]

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Natural attenuation is a commonly observed phenomenon in most contaminated sites.(Kao et al. 2010; Kawabe and Komai 2019) Natural attenuation describes naturally occurring processes in soil and groundwater that lead to a reduction in the mass, toxicity, mobility, volume, or concentration of contaminants without human intervention.(Jin et al. 2020) Natural attenuation combined with long-term monitoring (known as monitoring natural attenuation, MNA) has been proven to be a resultful remediation technology in petroleum-contaminated sites in which the biodegradation was the mainspring study conduct at contaminant removal.(Chiu et al. 2013; Naidu et al. 2010) Trends analysis and prediction are important segments for MNA application, in which complex biotic and abiotic factors need to be considered.

Microbiome data has been shown to work in combination with machine learning in parsing or predicting the degradation process of organic pollutants.(Bellino et al. 2019; Wijaya et al. 2023) Microbial communities acclimatized themselves to the local physicochemical conditions as well as to the pollutants in a historically contaminated site.(Guo et al. 2019; Yu et al. 2023; Sperlea et al. 2022) Due to their susceptivity to discrepancies of their surroundings, microorganisms could be regarded as "first responders"to environmental changes.(Sperlea et al. 2022) The microbial information carries additional information about environmental conditions and should be of great advantage in simplifying natural attenuation predictions, but there are few reports on this area.

In this work, the long-term monitoring of BTEX/CAHs and microbial community in the groundwater of a pesticide plant was conducted. A machine learning approach for natural attenuation prediction was developed with RFC model followed by either RFR or ANN model, utilizing both microbial information and contaminant attenuation rates for model training and cross-validation. The performance of the models in the prediction of the feasibility and/or rates of natural attenuation of BTEX and CAHs was subsequently evaluated and compared.

Results showed that the RFC model could achieve high accuracy (above 99%) for the feasibility prediction of natural attenuation for both BTEX and CAHs, and could successfully identify the key functional microbial genera. The RFR model was sufficient for BTEX natural attenuation rate prediction, and the MAPE was 8.1% ~ 19.6%. However, the predicted natural attenuation rates of CAHs by RFR were unreliable, with the MAPE as high as 22.0% ~ 153.9%. The ANN model showed better performance in the prediction of attenuation rates for both BTEX (with MAPEs from 2.1% to 4.6%) and CAHs (with MAPEs from 6.9% ~ 19.7%). Based on the assessments, a composite modeling method of RFC and ANN models was proposed, which could reduce the MAPE to as low as 2.1% ~ 4.6% for BTEX and 6.9% ~ 19.7% for CAHs. This study reveals that the combined machine learning approach under synergistic use of site microbial data has promising potential for predicting natural attenuation.

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MS12 / 645

Interaction Mechanism Between Hydrate Phase Transition and Deformable Sediment Structure under Cold Seep System

Author: Xuan Kou[None]

Co-authors: Xiao-Sen Li [1]; Yi Wang [1]

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Cold seeps under seafloor manifests the migration of methane-rich fluid from the sedimentary subsurface to the seabed and into the water column, and even reach the atmosphere. As an important way of methane cycling on the Earth, the cold seeps are often accompanied by the occurrence of methane hydrates, which are hydrocarbons resources with the high hydrogen to carbon ratio. However, the interaction influencing mechanism between methane hydrate phase transition and methane-rich fluid (particularly methane gas) seepage in deformable subsurface marine sediments

are still lacking knowledge. In this work, we conducted in-situ hydrate formation and dissociation experiments in fine grained clayey sediments collected from the active cold seep area in South China Sea. By advanced X-ray Computed Tomography technology and in-situ heating as well as hydrate phase transition controlling method, we successfully acquired the dynamic hydrate phase transition behaviors and its effects on sediment pore structure evolution, anisotropy methane seepage, and solid migration under complex thermo-hydro-mechanical conditions. It is revealed that methane hydrates first occupy initial sediment pores while generating new pores and fractures in clayey sediments. The filling and generation of pores by hydrate formation and growth lead to the pore morphology evolution. However, we found that the degree of anisotropy decreases while the fractural dimension increases with the growth of hydrate in pores. Meanwhile, hydrate formation results in solid (e.g. sediments and shells) migration, thereby leading to the pore structure transformation. The shape factor of pores increases with hydrate formation and decreases with hydrate dissociation. During hydrate dissociation, we found that hydrate tend to be reformed in clayey sediments before initiating dissociation. The combining effects of hydrates reformation and hydrate dissociation lead to more enlarged pores in sediments. More significantly, the enlarged pores result in unpredictable damage to the sediment structure after the termination of hydrate dissociation. To address this potential poromechanical problem, we further simulate the solid migration process in clayey sediments during the overall hydrate phase transition process. It is found that the solid particles migrate toward the bottom of the sediments during hydrate formation process, leading to the compaction of sediment structure. On the contrary, during hydrate dissociation, the solid particles significantly move toward the upper region of the sediment, as the results of gas and water seepage through the newly generated and enlarged pores. These experimental observations would improve our understanding of the poromechanical controls and influencing mechanisms between hydrate phase transition, pore structure evolution, and hydrocarbon fluid flow in cold seep systems.

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MS04 / **648**

Impact of dynamic pore structure on local macroscopic parameters

Author: Jing Chen[None]

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In continuum models for drying, macroscopic parameters are integral, relying on the microstructure of porous media. These parameters are determined through the volume averaging of state variables, often derived from simulations using fixed pore network models (PNM). While fixed PNM is

a prevalent computational method, it typically assumes a static microstructure throughout the drying process, neglecting the dynamic changes inherent in drying deformable porous media. These changes significantly alter both the structural and transport properties of the porous medium. This study introduces an adaptive pore network model developed to capture the dynamic microstructure and mass transport kinetics of a model capillary porous medium under slow drying conditions. Through adaptive PNM simulations, key parameters, including local relative humidity and moisture transport coefficient, are derived. The findings reveal that, particularly in the later stages of drying, the non-local equilibrium effect becomes pronounced, evidenced by the deviation of local vapor pressure from equilibrium vapor pressure. Moreover, the moisture transport coefficient is primarily influenced by the liquid phase, leading to an extended transport region where the process dynamics are mainly governed by the presence and movement of liquid. This adaptive approach provides a detailed view of how microstructural changes interact with local macroscopic parameters during the drying of deformable porous media.

Acknowledgement

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Poster / 649

Digital-rock simulation of stress-dependent porosity and permeability for carbonate rocks

Authors: Ziyi Pu[1]; Ye Tian[1]; Yangyang Lei[2]; Yi Yang[1]; Ying Li[1]; Yulong Zhao[1]

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During fluid production or injection, the reservoir rock undergoes deformation due to the temporal variations of the effective stress field, which can alter the rock porosity and permeability, and further affect the reservoir performance. Previous digital rock models primarily emphasized the quantification of rock properties of the original core, meanwhile often neglecting the alterations of rock properties under dynamic stress. For example, the stress-dependent porosity and permeability are often ignored, leading to disparities between the actual rock measurement and the values calculated by the digital rock models. Carbonate reservoirs exhibit significant heterogeneity in pore distribution, hence it becomes imperative to conduct post-compaction simulation of the stress-dependent properties for carbonate rocks.

Based on the digital rock methodology, our study constructed digital rock models using the real data from carbonate rock CT scan. The median filtering method was employed for noise reduction. Subsequently, simulation of uniaxial compression was conducted. Firstly, the solid mechanics simulation was performed to simulate the deformation of the rock matrix within the core after compression under various stress conditions (e.g., changing the confining stress under the constant axial stress). The digital rock models after compaction were then constructed. Secondly, the separation of the rock skeleton and pores was executed for the compressed rock as shown in Fig. 1. Then, the pore mesh model was reconstructed and gridded to generate a digital model exclusively containing the pores as shown in Fig. 2. Following this, the fluid dynamics simulation was carried out to obtain the porosity and permeability data of the rock after stress-induced deformation and finally, the evolution law of rock porosity and permeability to the effective stress.

The rock strain analysis reveals that the stress-induced deformation primarily occurs within the fractures of the fractured rocks. The rock skeleton undergoes minimal changes, and the fixed constraint surface (bottom surface) remains stationary, with displacement intensifying closer to the axial compression loading surface (the top surface in Fig. 3), as the external load increases, the changes of the rock become more obvious. The stress concentration phenomenon occurs at the interface between the skeleton and pores. The closer to the pores, the more pronounced this stress concentration becomes. Specifically, at the same height, the displacement of the pores after compression is consistently the largest, and the overall deformation of the rock is more significant in the middle and smaller on both sides. In places with a high degree of tortuosity, the flow velocity is relatively small as shown in Fig. 4. Our calculation shows as the external loads increase, the porosity and permeability would decrease, showing a nearly linear decreasing trend.

In this study, we established an improved digital rock model considering the stress-dependency effect and calculated the porosity and permeability under varying stresses through the coupled simulation of fluid dynamics and solid mechanics. This provides the theoretical foundation for a more accurate description of the formation properties after fracturing. Simultaneously, it offers insights that can guide the computation of properties for other porous rocks, such as tight sandstone and shale.

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Poster / 650

Research and evaluation of damage mechanism of pore scale water phase trap in tight sandstone gas reservoir based on numerical simulation

Authors: Mingjun Chen[1]; Xingyu Tang[1]; Yili Kang[None]

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Background, Aims and Scope.
Tight gas resources are abundant and widely distributed, which is an important part of unconventional gas exploration and development. However, the tight sandstone reservoir has the characteristics of low porosity and permeability and micro-fracture development, so the water phase trap damage is more serious in the process of reservoir reconstruction. In addition, it is difficult to evaluate the damage of water phase trap in tight sandstone gas reservoirs at pore scale, and it is impossible to make a more accurate judgment of flowback and production pressure difference, which restricts the development of tight gas. Therefore, this study has practical guiding significance for the efficient development of tight sandstone gas reservoirs.
Methods.
Through core NMR experiments and finite element numerical simulation, the spatial and temporal distribution of water saturation and pressure in the pore throat of the gas-water phase in the process of forced imbibition and flowback is verified. The water phase trap damage degree of tight sandstone gas reservoirs at micro scale is evaluated by treating the part of the flowback model higher than the specific water saturation as the matrix.
Results and Discussion.
(1) In the process of forced imbibition, the high pressure area mainly concentrated in the blind end and narrow throat; The liquid phase flows rapidly through the dominant channel, and after a period of time, the distribution of pressure and water saturation in the whole system tends to be stable. (2) After flowback, a large number of isolated bubbles appeared in the capillary channel, which increased the frequency and severity of the occurrence of Jamin effect, resulting in a large amount of fracturing fluid remaining in the pore throat; (3) The calculated results of the model are basically consistent with those of core NMR. (4) The permeability of the two models before and after imbibition reflux was calculated respectively. The permeability of the model after imbibition reflux was significantly lower than that of the model before imbibition.

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MS23 / 651

Bridging the Gap: Connecting Pore-Scale and Continuum-Scale Simulations for Immiscible Multiphase Flow in Porous Media

Author: Mohammad Ebadi[1]

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Our work aims to bridge length scales in immiscible multiphase flow simulation by connecting pore-scale and continuum-scale simulations through a novel validation framework. We employ Niessner and Hassnaizadeh's (2008) continuum-scale model for multiphase flow in porous media, combined with McClure et al.'s (2020) geometric equation of state, to provide a complete set of geometrical measures. Pore-scale fluid configurations simulated with the Lattice-Boltzmann method are used to validate the continuum-scale results. We propose a mapping from the continuum-scale to pore-scale utilizing a Generalized Additive Model to predict non-wetting phase Euler characteristics during imbibition, effectively bridging the continuum-to-pore length scale gap. Other continuum-scale simulated measures of specific interfacial area, saturation, and capillary pressure are directly compared to up-scaled pore-scale simulation results. Overall, the proposed framework provides reasonable front profiles for saturation, capillary pressure, specific interfacial area, and Euler characteristic for an imbibition process.
The described workflow advances the modelling of immiscible multiphase flow by establishing a transparent connection between pore-scale and continuum-scale simulations, supported by fundamental thermodynamic and geometrical principles. Furthermore, the generated results for the Lattice-Boltzmann simulations demonstrate that utilizing the fluid configurations obtained from the outcomes of pore-scale simulations not only offers analytical references for validating the continuum-scale simulations but also serves as an interface to compare pore-scale and continuum-scale simulations. Future work remains for evaluating the extended multiphase flow model and our proposed framework for flow reversal processes such as drainage followed by imbibition.

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Poster / 652

Determination of gas content in shale by adsorption and desorption experiment

Author: Jian Guan[1]

Co-authors: Songyan Li [1]; Xiaobing Wang [1]

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Shale gas is a natural gas accumulation mainly located in shale rock series, with adsorption and free state as the main modes of existence, whose content directly affects the cumulative production, gas well's productivity and life, and is an important index for selection of exploration blocks and reservoir's evaluation. The determination methods of gas content in shale mainly include desorption method, isothermal adsorption and logging interpretation. In this paper, desorption method is adopted in production experiment with pressure reducing to study the gas content in shale. The

results show that the production process of shale gas can be divided into three stages, namely, the lost gas escaping stage, the rapid desorption stage and the slow desorption stage. The production rate is the highest in the initial stage of pressure-reducing production. After entering the stable production period, the gas production rate remains stable but the stable period is short, and then the gas production rate gradually decreases. The proportion of gas loss in shale decreases with the increase of pressure drop rate, accounting for 40%~50% on average, so the core should be lifted quickly during the coring process in the field to reduce the gas loss. In this paper, the experimental method of restoring shale to its original state and then producing with pressure reducing is helpful to improve the accuracy of gas content determination in shale, and can provide basis and reference for the actual exploitation of shale gas.

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Poster / 653

Preparation of municipal solid waste incineration (MSWI) fly ash-based self-foaming materials and feasibility study on goaf filling

Authors: 国胜付[1]; 森友安[1]

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As a toxic solid waste, the treatment and placement of MSWI fly ash has become a hot topic in society. It was found that the residual aluminum in MSWI fly ash reacted with the alkaline activator to generate hydrogen, which made the material present a pore structure without using the foaming agent. Using MSWI fly ash and coal gangue powder as the main raw materials, geopolymer foam materials with different ratios were prepared after alkali excitation. The effects of curing temperature, activator dosage and MSWI fly ash content on the compressive strength, fluidity, heavy metal leaching concentration, phase composition and pore structure of filling materials were studied. The feasibility of the application of alkali-activated MSWI fly ash-based spontaneous foam material in the filling work of mine goaf was explored. The results showed that when the curing temperature increased from 20℃ to 40℃, the 28d compressive strength of the material increased by about 24.2 %. The increase of curing temperature can significantly improve the degree of polymerization and the solidification rate of heavy metals, so that more polymerization products were generated in the system and the conversion of calcium silicate hydrate (C-S-H) to calcium aluminosilicate hydrate (C-A-S-H) with higher degree of polymerization is promoted. At the same time, the curing temperature will also affect the pore structure of the material. The higher the temperature, the larger the porosity of the material, and the smaller the complexity of the spatial distribution of pores.
Keywords: MSWI fly ash; Self-foaming filling materials; Filling body; Curing temperature; Pore structure

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MS17 / **657**

Fluid solid coupling simulation of deep carbonate gas reservoirs based on digital cores

Authors: Ruihan Zhang[1]; Tingting Wu[2]; Yulong Zhao[1]; Deliang Zhang[2]

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Carbonate gas reservoirs play an extremely important role in global natural gas resources, accounting for approximately 60% of total natural gas production. In recent years, deep carbonate gas reservoirs have become an important area for increasing global storage and production. However, deep carbonate gas reservoirs are buried deep, tight, high-temperature and high-pressure, with diverse types of storage spaces and strong heterogeneity. The flow behaviors under the stress strain mechanism during the production process are unclear, making it difficult to formulate reasonable production systems. To address the aforementioned issues, this article utilizes CT scanning and digital core reconstruction techniques to finely construct 3D digital cores for different reservoir space types such as fracture type, fracture-pore type, and pore-vuggy type. Based on the Darcy Biot fluid structure coupling method, a mathematical model is constructed to couple the flow equations and stress-strain control equations of the matrix, fracture, and vuggy system, and numerical solutions are obtained using the VOF method. Finally, conduct analysis of the influencing factors such as different storage space types, production systems, and reservoir physical properties on fluid flow behaviors and stress-strain distribution characteristics.

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MS11 / 658

Influence of fluids properties and pore-throat structure on snap-off: microfluidic experiments and theoretical analysis

Author: Bei Wei[1]

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The snap-off phenomenon occurs when a non-wetting phase flows from a water-wet constriction into a pore filled with water, resulting in the separation of the non-wetting phase into droplets. This phenomenon is commonly observed in various fields such as petroleum development, chemical engineering, and carbon utilization and storage. Numerous studies have investigated the underlying mechanism and identified critical capillary numbers associated with snap-off. However, there is a limited amount of research that specifically examines the impact of fluid viscosity and pore-throat structure parameters on this phenomenon.

In this work, we study the snap-off process when the oil droplet passing through the microchannel with a rectangular cross-section. The microfluidic chips are made of PMMA and have different constriction widths, heights, and lengths. By compounding silicone oil with different viscosities, we were able to modify the viscosity of the non-wetting phase. Through microfluidic experiments, we analyzed various snap-off patterns. Furthermore, we constructed a phase diagram illustrating the snap-off behavior under diverse oil viscosities and pore throat structural parameters.

The findings demonstrate that there is an inverse relationship between the viscosity of oil and the critical capillary number of snap-off, as well as the range of capillary numbers associated with snap-off. This can be attributed to the fact that the viscous force hinders the snap-off. When the capillary number reaches a certain threshold, the oil flows through the pore throat rapidly, preventing the water film from adequately entering the throat to establish a force equilibrium. The capillary number range associated with snap-off expands as the throat length and depth increase. Snap-off is observed only when the throat depth surpasses a specific threshold value. In addition, the capillary number does not influence the size of daughter droplets, and they are approximately 1.3-1.5 times the diameter of the throat. This investigation could help control the snap-off occurrences in engineering scenarios through the manipulation of fluid parameters and capillary structure.

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Pore-scale modelling of CO2 transport in saline aquifer of South China Sea and its influencing factors

Authors: Jia Zhao[None]; Chuanjin Yao[None]; Yuyuan Song[None]; Yiran Zhou[None]; Xiuqing Zhang[None]; Jiaqi Zhong[None]

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The instability associated with CO2 transport in porous media has a profound impact on geological carbon sequestration. A comprehensive depiction of the CO2-brine displacement process at the pore scale is indispensable for a nuanced comprehension of macroscopic processes at the continuum scale. This study integrated the structural features of the HJ saline aquifers in South China Sea with numerical simulations to scrutinize the transport of CO2-brine in porous media. The influences of capillary number (Ca), viscosity ratio (M), and wettability on CO2 phase saturation, phase interface evolution, and fingering phenomena within the pores were meticulously analyzed. The research unveiled that at lower Ca, the displacement manifested multiple loosely connected or disconnected finger flow paths. With an increase in the Ca, the fingering pattern evolved from capillary fingering to viscous fingering, resulting in an approximately 36.3% higher CO2 saturation when viscous forces dominate compared to capillary forces. Maintaining a constant injection velocity, the impact of M on displacement stability was relatively modest, primarily concentrated in the initial stages of displacement. Appropriately decreasing M can enhance CO2 saturation during stable displacement. Changes in wettability significantly affected displacement stability, CO2 transitioned from dispersed fingering to cluster-driven displacement as the medium gradually becomes less hydrophilic, leading to a 39.1% increase in CO2 saturation. This study furnishes theoretical insights for evaluating the efficacy of CO2-brine sequestration and enhancing storage methodologies.

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Poster / 661

Sub-core scale investigation of heterogeneity effect on CO2 transport in natural conglomerate cores

Authors: Xueqing Zhou[1]; Linqi Zhu[1]; Yuan Chen[1]

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To assess the impact of complex heterogeneities in conglomerate on pore distribution and fluid flow, the effect of heterogeneous debris spatial distribution in conglomerate on CO2 migration under reservoir conditions was studied using X-ray Computed Tomography (X-CT). Four types of conglomerate cores were drilled from the CO2 storage site in the Fushan Depression, China, which include uniformly distributed clasts sandstone, layered clasts, mud-bearing interlayered sandstone, and sandstone. These four conglomerate cores, characterized by different distributions of matrix and clasts, represent highly heterogeneous features. We conducted two-stage sub-core scale flow experiments. Drainage and imbibition tests were carried out under reservoir conditions, with a focus on the impact of heterogeneity on CO2 distribution. We used CT to quantify the detailed process of residual and dissolution capture in heterogeneous rocks caused by clasts presence, which can be widely applied in areas such as CO2 sequestration and enhanced hydrocarbon reservoir exploitation.

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MS01 / 662

Minimum miscibility pressure determination in confined nanopores considering the presence of the second liquid phase

Author: Zhuo Chen[1]

Co-authors: Ruixue Li [2]; Jialin Shi [3]

[1] *University of Alberta*

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In recent years, tight and shale reservoirs have become increasingly significant in global oil and gas production. However, the recovery efficiency from these reservoirs remains low, with a substantial portion of shale oil left unrecovered. CO2 flooding has emerged as a leading method for enhanced oil recovery (EOR) in these environments, offering both improved oil extraction and opportunities for

Carbon Capture, Utilization, and Storage (CCUS), which could help mitigate global warming. A common characteristic of such reservoirs is the prevalence of nano-scale pores. Accurately predicting the Minimum Miscibility Pressure (MMP) of oil and CO2 is vital for the successful implementation of CO2 injection strategies in unconventional reservoirs. However, existing MMP prediction methods are primarily developed for bulk conditions and fail to accurately predict MMP in the nanopores common in tight/shale reservoirs. Furthermore, modeling the oil-CO2 MMP in shale reservoirs is complicated by the frequent occurrence of vapor-liquid-liquid (VL1L2) three-phase equilibria, where the L1 phase represents the heavier liquid phase, and the lighter liquid phase (L2) contains a significant amount of gaseous solvents. The presence of this second liquid phase can significantly affect oil recovery efficiency and CO2 storage capacity due to changes in relative permeability curves and MMP values.
This paper presents the development of a comprehensive thermodynamic model that more accurately describes oil-CO2 MMP profiles in tight/shale reservoirs, taking into account the presence of the second liquid phase. A novel MMP calculation algorithm, based on the MMC algorithm, is introduced, incorporating the effects of capillarity, confinement, and the second liquid phase. Example calculations demonstrate the effectiveness and the robustness of the proposed algorithm. The results indicate that the confined oil-CO2 MMP decreases with diminishing pore radius, a trend more pronounced in smaller pores. Beyond a pore radius of 10 nm, the confined MMP becomes less sensitive to radius changes. Additionally, for each pore radius, the confined oil-CO2 MMP initially increases then decreases with rising temperature, suggesting a maximum MMP at a specific temperature. There is also a maximum confined MMP for each pore radius at the given temperature, which decreases with smaller pore radius. Additionally, the calculated MMPs considering the presence of the second liquid phase is larger than that without this consideration.

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Local thermal non-equilibrium processes influenced by interfaces within porous media systems

Authors: Anna Mareike Kostelecky[1]; Rainer Helmig[1]

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Non-equilibrium heat transfer processes across interfaces are of relevance in various environmental and technical applications, such as evaporation from soil, turbine blade cooling, geothermal energy systems and fuel cells.

For REV-based models, simplifications are necessary when accounting for local thermal non-equilibrium processes, as shown in Nuske et al 2. These simplifications strongly depend on interface-driven processes, such as the heat transfer from one phase to another phase. To describe heat transfer across different phases within the porous medium more accurately, an implicit, coupled pore-network model, so-called dual-network model 1, is extended. This model couples a network for the void space to a network for the solid phase of the porous medium to include effects of local thermal non-equilibrium processes. The analysis of local thermal non-equilibrium within the porous medium and towards the interface with a free-flow system is conducted using these models.

Our presentation will outline the current developments on how to include local-thermal non-equilibrium in pore-network and REV-based models. Additionally, we will present a comparison study between a dual network model and REV-scale model for single-phase systems. Furthermore, we provide brief insights on how current models can be adapted for multi-phase flow systems to account for heat transfer across different interfaces.

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1 Timo Koch et al. "A (Dual) Network Model for Heat Transfer in Porous Media: Toward Efficient Model Concepts for Coupled Systems from Fuel Cells to Heat Exchangers". en. In: Transport in Porous Media 140.1 (Oct. 2021), pp. 107–141. issn: 0169-3913, 1573-1634. doi: 10.1007/s11242- 021-01602-5. url: https://link.springer.com/10.1007/s11242-021- 01602-5 (visited on 12/27/2022)., 2 Philipp Nuske et al. "Modeling two-phase flow in a micro-model with lo- cal thermal non-equilibrium on the Darcy scale". In: International Jour- nal of Heat and Mass Transfer 88 (2015), pp. 822–835. issn: 0017-9310. doi: https : / / doi . org / 10 . 1016 / j . ijheatmasstransfer . 2015 . 04 . 057. url: https://www.sciencedirect.com/science/article/pii/ S0017931015004275.

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MS06-A / 664

Minimal Surfaces in Mixed-Wet Bead Packs: Insights from 3D X-Ray Imaging

Authors: Min Li[1]; Sepideh Goodarzi[2]; Jiafei Zhao[1]; Branko Bijeljic[2]; Martin Blunt[2]

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The interfacial curvature of immiscible fluids within porous media is critical for the comprehensive understanding of multiphase fluid, impacting capillary pressure, relative permeability, saturation distribution, and the formation of preferential flow paths. Despite many studies that have been made demonstrating that interfacial curvature is strongly affected by wettability, there are still some fundamental questions that remain unresolved. In this work, we employed three-dimensional (3D) X-ray imaging techniques combined with automated interfacial curvature analysis to examine the minimal surfaces under mixed wettability conditions, using random arrangements of spherical glass beads, which are hydrophilic, and plastic beads, which are hydrophobic. Our findings confirmed the existence of mean curvatures approaching zero (minimal surfaces), suggesting optimal conditions for the simultaneous flow of two connected phases. This work provides insight into the ideal wettability conditions for enhancing oil recovery, CO2 sequestration, hydrogen storage, groundwater remediation, optimizing water management in polymer electrolyte fuel cells, and designing microfluidic devices.

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MS17 / **665**

Temperature evolution law of mining coal seam in gas desorption process

Author: Wenlu Zhang[1]

Co-authors: Weiji Sun [1]; Bing Liang [1]; Jianfeng Hao [1]

[1] *Liaoning Technical University*

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In order to study the influence of coal desorption of gas heat effect and non-uniform boundary load on the temperature evolution law of coal and gas protrusion gestation process, we constructed the coal and gas heat-fluid-solid coupling model containing desorption of heat and carried out numerical simulation research. The study shows that: when considering the effect of desorption heat, the temperature changes in the stress elevation area, stress concentration area and stress unloading area have obvious stage changes, which can be divided into the pre-growth period, the middle period and the late period according to the rule of change. However, when the desorption heat effect is not considered, only the early and late stages of incubation exist; the effect of desorption heat promotes the temperature reduction of the coal body close to the working face, and inhibits the temperature reduction of the coal body far away from the working face; the non-uniform loading causes the temperature evolution of coal and gas protrusion process. The non-uniform loading causes the temperature in the stress concentration area of the coal seam to increase, and the value increases with the increase of the peak stress coefficient; the temperature drop of the coal seam decreases with the increase of the peak stress coefficient; heat convection and heat conduction are the main modes of

temperature transfer in the coal seam; the non-uniform loading causes the pore space of the coal seam to be tightly closed, so that the process of heat convection is blocked, while heat conduction is not easy to be affected. The results of the study clearly understand the influence of heat-absorption effect on the temperature of coal seams under the influence of mining stress, explain the reasons for the temperature changes in different stress zones of coal seams, and provide a reference for the research in the area of early warning of coal and gas protrusion.

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MS01 / **666**

Insight on the stability of gas hydrate in montmorillonite slits by molecular dynamics simulations

Author: Jie Chen[1]

Co-authors: Jiafang Xu [1]; Zhengcai Zhang [2]; Gaowei Hu [3]

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

[2] *Laoshan Laboratory*

[3] *Qingdao Institute of Marine Geology*

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The extent of interactions between clay surfaces and water molecules and their impact on hydrate stability in clay reservoirs have been a source of debate. This uncertainty arises from the inherent challenges associated with the nanoscale temporal and spatial detection of bound water molecule distribution characteristics. This study employs molecular dynamics simulations to investigate the stability of methane hydrates in montmorillonite slits at various temperatures, focusing on the surface influence scale, bound water molecule distribution characteristics, and binding strength. The results show that hydrates in close proximity to the clay surface exhibit lower stability and are more prone to decomposition. The hydrophilic nature of the surface leads to water molecule aggregation at the interface, driving methane molecules away during decomposition. Additionally, compared to the charged tetrahedral layer surface of montmorillonite, the quasi-liquid layer on the neutral tetrahedral layer surface is thinner, with semicage structures persisting within the vacancies of the Si-O rings. The analysis suggests that variations in the range of surface influence and binding strength can be primarily attributed to intermolecular Coulomb interactions and charge redistribution at the interface. These research findings offer valuable molecular insights into the microscopic characteristics and behavior of hydrates within clay slits.

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667

Experimental investigation on influencing factors of caprock breakthrough pressure under CO2 geological sequestration

Authors: Yuyuan Song[None]; Chuanjin Yao[None]; Xiuqing Zhang[None]; Jia Zhao[None]; Yiran Zhou[None]

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Geological carbon dioxide (CO2) storage offers a cost-effective solution for reducing CO2 emissions and mitigating climate change. However, the injection of CO2 into a reservoir can cause an increase in pore pressure, leading to fault reactivation or detrimental changes in the caprock. These changes can hinder the sequestration of injected CO2, especially when it comes to CO2 leakage through the caprock layer, including capillary leakage, hydraulic rupture, and leakage along pre-existing faults. Therefore, evaluating the confinement capability of the caprock is crucial for accurately predicting the long-term safety and stability of CO2 geological storage. One of the most essential parameters for characterizing the confinement capability of the caprock is the CO2 breakthrough pressure. It represents the minimum capillary pressure needed for the non-wetting phase to replace the wetting phase and establish a dominant seepage channel through the caprock. In this study, we conducted step-by-step experiments to determine the CO2 breakthrough pressure at the core scale. Additionally, we investigated how different factors such as caprock lithology, caprock thickness, and burial depth affect this pressure. The results of the experiments indicate that: 1) the permeability of the caprock layer is inversely proportional to the breakthrough pressure, meaning the lower the permeability, the higher the breakthrough pressure; 2) the CO2 breakthrough pressure increases nonlinearly with increasing caprock layer thickness; and 3) burial depth has a significant impact on the CO2 breakthrough pressure, which increases as the depth of burial increases. These findings provide a theoretical foundation for ensuring the safe and effective long-term stability of CO2 geological storage.

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MS22 / **668**

A combined ionic Lewis acid descriptor and machine-learning approach to prediction of efficient oxygen reduction electrodes for ceramic fuel cells

Author: Shuo Zhai[1]

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Corresponding Author: shuo.zhai@szu.edu.cn

Improved, highly active cathode materials are needed to promote the commercialization of ceramic fuel cell technology. However, the conventional trial-and-error process of material design, characterization and testing can make for a long and complex research cycle. Here we demonstrate an experimentally validated machine-learning-driven approach to accelerate the discovery of efficient oxygen reduction electrodes, where the ionic Lewis acid strength (ISA) is introduced as an effective physical descriptor for the oxygen reduction reaction activity of perovskite oxides. Four oxides, screened from 6,871 distinct perovskite compositions, are successfully synthesized and confirmed to have superior activity metrics. Experimental character- ization reveals that decreased A-site and increased B-site ISAs in perovskite oxides considerably improve the surface exchange kinetics. Theoretical calculations indicate such improved activity is mainly attributed to the shift of electron pairs caused by polarization distribution of ISAs at sites A and B, which greatly reduces oxygen vacancy formation energy and migration barrier.
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MS17 / **672**

Study the fluid flow interaction with fracture and matrix in the porous media.

Author: Kejian Wu[1]

Co-authors: Guan Qin [2]; Ciprian Panaitescu [3]

[1] *The University of Aberdeen*

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The research is to investigate the fluid flow dynamics during growth of fractures associated with matrix using direct observations from 3D computed tomography and microscale modelling approach. The lab experiment is carried out with both geomechanical and hydraulic experiment using rock core samples. The triaxial pressure, the flow rate as well as the pressure gradient are monitored throughout the experiment. The CT scanning imaging technology is an effective method that provides a direct information of pore/fracture structure, leading to multiscale fracture-matrix pore structure modelling and the flow simulation based on the interaction of pore/fracture fluid flow physics which can be validated by experimental data. The CT scanning and SEM images are used to build the fracture-matrix pore network model and the resultant flow simulations are calibrated with the lab data. The results of fracture-matrix modelling approach and calibration of flow simulation against measured data to reveal the interaction flow mechanism will be presented.

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MS06-A / 673

Pore-scale modeling of multiphase flow in porous media with particle migration

Author: Yuanping Li[1]

Co-authors: Hui Zhao ; Jingwei Huang ; Xiaolong Yin [2]

[1] *China University of Geosiences (Wuhan)*

[2] *Eastern Institute of Technology, Ningbo*

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Multiphase flow in porous media with moving particles is common in many natural and industrial processes, such as low-salinity water-flooding, sand production, and microbial enhanced oil recovery, etc. With complex interactions between fluids, particles and pore surfaces, the flow behaviors in such systems are often distinct. To understand the effects of particle migration on multiphase flow in porous media, a direct numerical simulation study is conducted. In this study, Navier-Stokes equation is coupled with discrete element method (DEM) by directly calculating fluid-particle interaction forces. The volume of fluid (VOF) method is used to capture the evolution of the immiscible

two-phase interface. Contacts between solid particles and pore walls with arbitrary topology are modeled by the contact laws. This study demonstrates that particle migration significantly alters the well-known characteristics of two-phase displacement, such as viscous fingering and capillary fingering. Particle plugging in the pore throat compels the invading fluid to enter larger pores, resulting in a higher sweeping efficiency. The role of particle density, injecting velocity, surface tension and other parameters are systematically analyzed. Finally, a mathematical model is established to describe the effects of particle migration on multiphase flow in porous media. The established model is validated against microfluidic experiments.

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MS15 / **674**

A neural network model with physics constraints for simulating CO2 storage in deep saline aquifers during and after injection

Author: Mengjie Zhao[None]

Co-authors: Yuhang Wang [1]; Marc Gerritsma [2]; Hadi Hajibeygi [2]

[1] *China University of Geosciences (Wuhan)*

[2] *TU Delft*

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The exploration of CO2 capture and storage has become a crucial element in strategies aimed at mitigating climate change, where deep saline aquifers are of particular interest due to their extensive storage capacity and widespread availability. The complexities involved in effectively monitoring and simulating CO2 behavior within these geological formations present significant challenges. To address these challenges, our research introduces a specialized neural network, designed to simulate and monitor CO2 storage in deep saline aquifers during both the injection and post-injection phases. This neural network represents an integration of physics-based principles and advanced deep learning techniques. This integration facilitates the modeling of CO2's complex movement and distribution under diverse conditions. The network's ability to process and analyze spatial data, coupled with key geological characteristics, significantly enhances the accuracy of its simulations. This aspect is crucial for understanding the heterogeneous nature of subsurface systems and the dynamic behavior of CO2. The architecture of this network, encompassing various computational layers and physics-informed constraints, is designed to ensure comprehensive and precise modeling of CO2 storage processes. This approach aims to contribute to the existing body of knowledge in the field of carbon capture and storage, offering a new perspective in the simulation and understanding of CO2 behavior in subsurface systems.

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MS03 / **677**

Wettability Impact on Immiscible Fluids Flow in Rough Fracture

Author: dongsheng wu[1]

Co-authors: Han-Xing Deng [1]; Xiao-Guang Wang [1]; Dong-Po Wang [1]

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Wettability can dramatically impact on the immiscible fluids flow in permeable media, including subsurface technologies to microfluidics. Previous studies have profoundly revealed this effect on flow in porous media, but so far, few systematic results on how the wettability controls flow in rough fracture are reported. Here, we conduct the visualization experiment to investigate the immiscible fluid-fluid displacement, by systematically varying the wettability of the fracture cell over a wide range of contact angles. Our observation shows that increasing the fracture's affinity to the invading fluid results in more efficient displacement of the defending fluid up to a critical wetting transition, beyond which the trend is reversed. We find this critical contact angle is related to the roughed-wall geometry. We derive a theoretical model that describes the transitions of displacement patterns from capillary imbibition to capillary fingering to the crossover to viscous fingering as functions of wettability. This work draws the phase diagram considering wettability in rock fracture and is of practical significance in subsurface applications.

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MS13 / **678**

A Modified Simplified Local-Density Model for Gas Adsorption Considering Cylindrical Pore Structures

Author: Jialin Shi[1]

Co-authors: Zhuo Chen [1]; Ke Hu [1]

[1] *University of Alberta*

Corresponding Authors: kh10@ualberta.ca, jialin4@ualberta.ca, zhuo8@ualberta.ca

Recent developments in unconventional oil and gas reservoirs such as shale gas have brought the pore structures and gas adsorption characteristics into focus. Traditional models, such as the original Simplified Local-Density (SLD) model with a slit-shaped pore, fall short in accurately describing gas adsorption in these reservoirs due to the presence of various carbon pore geometries, including slit and cylindrical shapes. In this study, we develop a modified SLD model, specifically adapted for circular shale nanopore geometries. Such model, based on cylindrical pore structures, incorporates a modified attractive parameter to account for the curvature effect on gas adsorption behavior. We validate the model's efficacy by examining the isobars and isotherms of methane over a wide range of temperature and pressure in various cylindrical pores.

The results demonstrate that the adsorption isotherm and density profile calculated by the modified SLD model are in strong agreement with experimental data. Furthermore, such modified model effectively captures the methane adsorption isotherm observed in shale, demonstrating its superior capability in characterizing pore structures within unconventional gas reservoirs.

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Poster / **679**

TH2M modelling: Extended analysis of gas phase appearance in low-permeable porous media

Authors: Norbert Grunwald[1]; Olaf Kolditz[2]; Michael Pitz[3]; Thomas Nagel[4]

[1] *UFZ*

[2] *Helmholtz Centre for Environmental Research UFZ / TU Dresden*

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This manuscript presents a comprehensive study on the numerical simulation of gas transport in clay rock using the finite-element method, with a specific focus on the transition of the transport regime from single-phase to two-phase conditions. Our code demonstrates the capability to cover this transition seamlessly, without relying on common approaches such as the use of persistent primary variables or the switching of primary variables. In our simulations, the primary variables are gas pressure, capillary pressure, temperature, and displacement of the solid phase. To validate our approach, two benchmark tests were conducted. The first benchmark replicates a well-known scenario in the field of radioactive waste disposal, where gas injection induces a transition from single-phase to two-phase flow. The second benchmark simulates a core drilling experiment, where the mechanical unloading of a fully saturated domain results in the appearance of a gas phase. In addition to analyzing primary quantities, a comprehensive set of secondary variables was introduced to gain deeper insights into the model's operation and enhance understanding of the underlying processes. By plotting these secondary variables alongside the primary quantities, a comprehensive understanding of the system's behavior during the transition of flow regimes was obtained. The primary objective of this work is to improve our understanding and confidence in the model used for simulating large repository systems, particularly in the context of nuclear waste disposal and CO_2 storage. By successfully capturing the transition from single-phase to two-phase gas transport, our study provides valuable insights into the behavior of gas in clay rock. This enhanced understanding lays the groundwork for utilizing the model effectively in large-scale repository simulations, contributing to the advancement of the field of gas transport in clay rock.

Source:
Grunwald, N., Nagel, T., Pitz, M., & Kolditz, O. (2023). Extended analysis of benchmarks for gas phase appearance in low-permeable rocks [Article]. Geomechanics and Geophysics for Geo-Energy and Geo-Resources, 9(1), Article 170. https://doi.org/10.1007/s40948-023-00703-3

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MS09 / 681

The interplay between temperature evolution, species distribution, and microstructure dynamic in a calcining porous particle

Authors: Xiang Lu[None]; Jing Chen[None]; Abdolreza Kharaghani[1]

[1] *Otto von Guericke University*

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Reacting particle systems play a crucial role in various industrial applications, with limestone calcination serving as a prime example. In this process, applying high-energy input to calcium carbonate ($CaCO_3$) particles results in the production of active lime solid (calcium oxide CaO) and the by-product carbon dioxide (CO_2) gas. The legal obligation to mitigate CO_2 emissions has a notable impact on production costs, emphasizing the need for a thorough understanding of the calcination process. Such an understanding can enhance conversion process efficiency and enable the achievement of desired CaO structures, crucial for high efficiency in CO_2 adsorption. This study introduces a pore network model to explore the interplay between intraparticle heat and mass transfer, pore structure changes during chemical reactions, and their interactions with the surrounding fluid-solid environment in a single particle. The pore space and solid skeleton of the particle are approximated as regular-lattice networks, incorporating cylindrical pores and volume-less nodes. Local reaction rates are determined based on the effective specific surface area and local CO_2 pressure. Thermal energy is supplied through hot gas flow convection at the network's surface. Solid element dimensions and corresponding pore structures are updated during each time step, enabling the tracking of temperature evolution, local conversion, and void space structure changes within the particle. Simulation results reveal that when the bulk gas has initially low CO_2 pressure, calcination extends beyond the particle surface and occurs within the particle. As a result, the released CO_2 becomes trapped due to internal mass transfer resistance, impeding further calcination. On the contrary, exposure to high initial CO2 pressure exclusively promotes local calcination reactions at the particle's surface. The initial bulk CO_2 pressure also has a notable impact on the final structure of CaO. This intricate interplay in calcination, as demonstrated by the simulations, provides valuable insights for a better understanding and optimization of industrial processes, applicable not only to calcination but also to other heterogenous reactive systems.

Acknowledgement

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Poster / 682

Characterization of Fluid Mobility and Determination of Movable Pore Throat Lower Limit in Deep Tight Sandstone Reservoirs Based on Nuclear Magnetic Resonance

Author: Yuchao Wang[1]

Co-authors: DongXia Chen [1]; Fuwei Wang [1]

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Study on the Fluid Mobility Within Reservoir Microscopic Pore Throats Holds Significance for the Precise Evaluation of Reservoirs and the Efficient Development of Oil Fields. Nuclear magnetic resonance can rapidly and accurately determine common movable fluid parameters such as movable fluid saturation, movable fluid porosity, and bound fluid saturation. This enables effective fluid assessment and productivity prediction for various types of oil and gas reservoirs. In this research, different facies' sandstone fluid mobility and the lower limit of movable pore throats in lacustrine delta-turbidite systems were characterized via multi-gradient centrifugation nuclear magnetic resonance. This study, combined with experiments including particle size analysis, thin sections, X-ray diffraction, and high-pressure mercury tests, explicitly delineates the impacts of reservoir deposition, diagenesis, reservoir type, and microscopic pore structure on movable fluid saturation. The research findings reveal three types of lithofacies, three categories of pore throat structures, and three classes of pore throat spaces (micropores, sub-micropores, and nanopores) in the study area. Micropores and sub-micropores are prevalent in blocky and laminated fine sandstones of the delta front facies, with higher fluid migration rates in micropores than in sub-micropores, and nanopores exhibit the lowest rates. Turbidite facies mudstone fine sandstone and calcareous fine sandstone contain sub-micropores and nanopores, showing the highest fluid migration rates in sub-micropores. Fluid mobility is influenced by various factors such as rock physical properties, diagenetic minerals, pore-throat structures, and lithofacies. As pore-throat structures and petrophysical properties deteriorate, the fluid mobility in all three types of reservoirs decreases. The movable fluid content shows a significant correlation with feldspar content, highlighting the improved fluid mobility of feldspar dissolution pores. Conversely, carbonate minerals and clays (plastic minerals) exhibit a negative correlation with movable fluid percentage (MFP), resulting in reduced quality of reservoirs and pore structures. Additionally, the sand ratio (sandstone thickness/formation thickness), sandstone layer thickness, and distance from source-reservoir boundary affect the movable fluid saturation. Thicker sandstones with lower mud content and carbonate cement show higher movable fluid saturation. Conversely, thin sandstones often embedded in thick mudstones exhibit higher carbonate and clay content at source-reservoir interfaces, leading to decreased movable fluid saturation. Moreover, with increased centrifugal force, micro-nano-pore fluid production initially increases rapidly and then stabilizes. Under 2.75 MPa, nanopore fluids migrate towards micropores, calculating a movable pore throat radius of 18nm~30nm. The research outcomes contribute theoretical references for understanding and effectively developing deep tight sandstone reservoirs.

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Poster / 683

Establishment and analysis of characterization model of oil-water flow energy consumption in porous media

Author: Yajie Bai[None]

Co-authors: Jian Hou ; Yongge Liu

Corresponding Authors: byj_819@hotmail.com, sllx_upc@126.com, liuyongge@upc.edu.cn

Due to the law of flow energy consumption in the porous media process is relatively vague, in order to effectively control the energy consumption in the process of oil production by water flooding, a characterization model of oil-water flow energy consumption in porous media during oilfields water flooding development is proposed. The influencing factors of reservoir energy consumption under different reservoir geological parameters and different production scheme are analyzed.Through fluid mechanics, the energy conversion relationship among potential energy, pressure energy and kinetic energy in the reservoir is studied. Through Bernoulli equation, the changes of water injection energy, oil production energy and formation elastic energy in reservoir are transformed into the changes of formation pressure. And the energy consumption characterization model of reservoir is established. Through the numerical simulation technology, the pressure, flow and velocity distribution of the reservoir are simulated, and the injection energy, the consumption energy and useless consumption ratio of the whole reservoir are calculated through the flow relationship in the reservoir.Firstly, the energy consumption characterization model of the reservoir subsystem is established by considering the injection energy, production energy and formation energy (potential energy, kinetic energy and pressure energy) of the reservoir system during oil production process. The oil-water flow energy consumption model in porous media is verified by different production systems in the ideal model. With the reservoir development by water injection, the water cut increases gradually, the proportion of energy consumption decreases gradually, but the energy consumption per tonne oil increases gradually. Then, the influence of geological parameters such as permeability and viscosity on energy consumption of reservoir system is considered. Under the same water cut, the energy consumption and its proportion of reservoir system increase with the decrease of permeability and the increase of viscosity. In addition, under the low permeability and high viscosity, the proportion of energy consumption of reservoir is nearly 100%. Finally, the influence of production parameters such as well spacing on energy consumption of reservoir system is considered. Well spacing has little effect on the energy consumption and its proportion of reservoir system. Formation pressure has little effect on the energy consumption,but its proportion decrease with the increase of formation pressure.The characterization model of oil-water flow energy consumption in porous media can quantitatively represent the energy completely lost due to friction in reservoir. Study on the law of oil-water flow energy consumption in porous media can effectively improve production efficiency, reduce useless energy consumption and oil production costs.

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MS23 / 684

Competition between main meniscus flow and corner film flow in strongly wetting porous media: a pore network study

Author: Jianlin Zhao[1]

Co-authors: Dominique Derome [2]; Guangqing Zhang [1]; Jan Carmeliet [3]

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[2] *Universite de Sherbrooke*

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Wetting film can develop in the corners of pore structures during imbibition in a strongly wetting porous medium, which may significantly influence the two-phase flow dynamics. Due to the large difference in scales between main meniscus and corner film, accurate and efficient modeling of the dynamics of corner film remains elusive. In this work, we develop a novel two-pressure dynamic pore network model incorporating the interacting capillary bundle model to analyze the competition between main meniscus and corner film flow in real porous media. A pore network with four-point-star-shaped pore bodies and throat bonds is extracted from the real porous medium based on the pore shape factor and pore cross-sectional area, which is then decomposed into several layers of sub-pore-networks, where the first layer of sub-pore-network simulates the main meniscus flow while the upper layers characterize the corner film flow. The accuracy of the developed model is validated with lattice Boltzmann simulation of imbibition in a strongly wetting square tube and microfluidic experiments of imbibition in strongly wetting porous structures. Then the model is used to simulate imbibition in a strongly wetting sandstone porous medium and the competition between main meniscus and corner film flow is analyzed. Wettability is the most significant parameter controlling corner film flow. The wetting film can develop in the corner only when the contact angle is below a critical value. Under a constant capillary number and viscosity ratio, the corner film flow becomes more significant with the decrease of contact angle. For a small contact angle, a phase diagram characterizing the competition between main meniscus and corner film flow is proposed, dominated by the capillary number and viscosity ratio between wetting and non-wetting fluids. In general, with the decrease of capillary number and viscosity ratio, the wetting corner film flow becomes more significant. The snap off phenomenon caused by swelling of wetting corner film is also analyzed, which happens more frequently with the more pronounced wetting corner film. In addition, the frequency of snap off phenomenon increases with the size ratio between pore body and throat bond. This work deepens our understanding on the imbibition mechanisms under strongly wetting conditions, which provides basic theories for imbibition related engineering processes, such as geological carbon or hydrogen storage.

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Assessment of Fluid/Fluid Displacement in Mixed-wet Systems Using Microfluidic Devices

Author: Abdullah AlOmier[1]

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Assessment of the immiscible fluid displacement behavior in mixed-wet systems, such as carbonate and shale reservoirs, has gained a significant attention by the industry. Wettability of oil-brine-rock systems is a crucial petrophysical property that impacts fluid distribution and multiphase flow in hydrocarbon reservoirs. Microfluidics is a unique technology that can provide direct visualization and assessment of flow mechanisms at the pore scale. However, mimicking mixed-wet systems becomes a limitation to this technology. In this work, we investigate the influence of wettability on fluid/fluid displacement using microfluidic devices mimicking formations with single and mixed wettabilities for the first time.

The microfluidic devices were designed to replicate the actual pore-network of an oil-bearing reservoir rock, obtained from thin-section images of a core. The microdevices were built out of silicon due to their compatibility with organic solvents, such as oil. A novel technique was used to construct the microfluidic substrates with controlled wettability, including water-, oil-, and mixed-wet systems, imitating pore-network formations with variable pore-throats.

Multiple sets of comparative experiments were conducted to examine the influence of wettability on fluid displacement at the pore scale. Three silicon-based microfluidic devices were utilized, all featuring the same pore-network structure but differing in wetting characteristics. The first microdevice had a hydrophilic silicon-based surface without any surface modifications, simulating a water-wet system. The second microdevice had its surface fully coated with hydrophobic material, representing an oil-wet system. The third microdevice underwent selective wettability alteration by depositing a hydrophobic coating on specific zones, creating multiple hydrophobic spots on the surface to mimic a mixed-wet system. All flow experiments shared identical conditions. Results revealed distinct fluid displacement patterns among the cases. Significantly, the mixed-wettability condition demonstrated a substantial impact on both fluid saturation and injection pressure compared to purely water- and oil-wet cases. This emphasizes the necessity of accurately designed microdevices that mimic mixed-wet formations when assessing fluid displacement. Single-wetting state microdevices may lead to underestimations or overestimations of the displacement process.

This work presents an assessment of mixed wettability impact on fluid displacement using mixed-wet microfluidic devices demonstrated for the first time. Tuning the wetting state of the microdevices to mimic the mixed-wet characteristics of reservoir rocks can enhance the understanding of multiphase flow behavior and recovery mechanisms in mixed-wet reservoirs, including carbonates and shales.

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MS04 / 692

Predictive modelling of liquid ingress into disintegrating pharmaceutical tablets

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In pharmaceutical science, the disintegration process refers to the mechanical breakup of an intact tablet into small fragments to increase the surface area of the drug substance in contact with the dissolution medium 1. Within the pharmaceutical industry, the disintegration time, which is the time required to disintegrate a tablet until no palpable residues remain, has been employed as one of the critical quality attributes to ensure the bioavailability and efficacy of end products. Despite its significance and extensive studies on the process, a universally accepted and practically employed model to quantitatively describe the disintegration process remains elusive due to the intricate physiochemical interplay of the process, coupled with complex formulations and manufacturing conditions.

At the microscale, determining the propagation of a capillary driven flow requires a solid understanding of the capillary structure including its deformation over time. However, it is practically impossible to capture the complexity in sufficient detail using established analytical methods for pharmaceutical tablets. We instead studied the propagation of the liquid front within the porous matrix, recognising the role of the advancing liquid as the initiator of all subsequent phenomena. Employing the terahertz pulsed imaging (TPI) technique coupled to an open immersion setup allowed us to precisely monitor the in-situ location of the liquid front whilst controlling the influence from the experimental setup on the liquid flow 2. This approach successfully captured the liquid ingress profiles of complex formulation tablets and revealed two regimes of liquid propagation: 1) an initial rapid uptake regime and 2) a subsequent slower linear regime, which was rate-limiting in determining the disintegration time.

Our results suggest that the linearity in transport results from the synchronised propagation of the liquid front and the erosion at the interface in touch with the dissolution medium [3]. Consequently, we employed this mechanism to develop a predictive model for the disintegration process of pharmaceutical tablets where each regime was modelled as a time-evolving porous medium in terms of swelling and erosion and its terminal structure transitioning inward. Based on TPI measurements, the associated fitting parameters were extracted to quantify the mass transport behaviour of the two regimes and compared across different tablets. This methodology and modelling offers insights into the disintegration process of pharmaceutical tablets and shows potential applicability in understanding disintegration for a range of swelling and eroding porous media.

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MS13 / 694

Multiscale modeling of ion transport in water saturated nanostructures of clays

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Ion diffusion within clays is a fundamental process related to contaminant transport in groundwater and radionuclide migration in the context of nuclear waste disposal. Montmorillonite, one of the predominant minerals within bentonitic clays, exhibits distinguished physicochemical properties such as the ability to absorb water and ions, accompanied by underlying swelling. This behavior is primarily governed by the electrical double layer (EDL) effect at the nanoscale. In turn, these nanoscale interactions have a critical influence on the macroscopic transport properties in clays. In this study, a multiscale modeling technique was developed to combine molecular-scale and pore-scale modeling. At the molecular scale, a coarse-grained (CG) mesoscale model was used to generate the nanostructures of sodium montmorillonite, where ClayFF force-field atomistic montmorillonite platelets are equivalently represented by coarse-grained platelets including two types of particles: central nonhydrogen-bonded particles and edge hydrogen-bonding particles (1). At the pore scale, the lattice Boltzmann method (2) is used to solve the coupled Poisson-Nernst-Planck equations on GPUs to model the transport of ions in the nanostructures obtained by the CG mesoscale model. Since the variable charge of the edges of the montmorillonite platelets depends on the pH, an inhomogeneous surface charge density is employed as a boundary condition to obtain the electric potential distribution. Quantitative analyses carried out by this multiscale model were implemented to investigate the influence of clay density, ionic strength, and pH on the effective diffusivities of ions. The insights into the ion transport process and the effect of edge sites in clays gained in this study can be implemented in larger-scale analyses such as continuum-scale reactive transport simulations for radionuclide migration in deep geological repositories for radioactive wastes.

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MS03 / 695

Pore-scale Modeling of Two-Phase Fluid Flow in the Fracturing-Shut In-Flowback Process of Tight Oil Reservoirs

Authors: Fangzhou Liu[1]; Daigang Wang[1]; Zhe Hu[1]; Kaoping Song[1]; Jin Chen[1]

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The storage space of tight formation after volumetric fracturing is complex, characterized by the coexistence of micro-nano pores and multi-scale fractures. This complexity hinders a clear understanding of pore-scale flow dynamics in the integrated fracturing-shut in-flowback process of tight oil reservoir. To tackle this issue, we introduced the micro-focus CT imaging and digital image processing technology to establish two digital rock geometry models retrieved from raw CT images. Subsequently, we proposed a pore-scale modeling workflow based on the pseudo- potential lattice Boltzmann model to explore the underlying mechanism of fluid exchange during the integrated development period. This workflow allowed us to investigate the oil-water exchange behaviors during the three stages of fracturing-driven, shut-in imbibition and flowback production. Ultimately, we conducted a systematic analysis of the influence of oil-water viscosity ratio, rock wetting angle and capillary number on the pore-scale oil-water exchange. Results show that during the fracturing-driven stage, fracturing fluid primarily migrates along the fractures, with only a small amount entering the pore space nearby the fractures. In the shut-in imbibition stage, the fracturing fluid preferentially flows into small pores, displacing the recovered oil droplets through the large pores. In the flowback production stage, oil droplets occupied in the fracture-matrix contact areas are preferentially stripped off, and there still exists a large amount of crude oil droplets that are difficult to be swept. A higher capillary number and a lower oil-water viscosity ratio will supply formation energy during hydraulic fracturing in tight oil reservoirs, activating the mobilization of crude oil droplet trapped in the stimulated reservoir volume region and improving imbibition recovery. The effect of wetting angle on energy supply during hydraulic fracturing in tight oil reservoirs is relatively little, while a higher water-wet degree will promote spontaneous imbibition, making it challenging for fracturing fluid to flowback.

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MS17 / **696**

Application of Automated Mineralogy in Fluid-Solid chemical reactivity transmission on reservoirs

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Automated mineralogy (AM) is a semi-automatic mineralogical tool based on a scanning electron micrography-energy dispersion spectrometry (SEM–EDS) platform. It has the functions of large-area high-resolution field image scanning, particle mineralogical analysis, specific mineral search, trace mineral search and so on. It can realize the identification and quantification of core minerals, surface porosity and pore morphology, mineral particle size and pore distribution characteristics, element occurrence form and so on. Therefore, AM data can be used to analyze the sedimentary environment and diagenetic evolution process of oil and gas reservoirs and even to evaluate oil and gas reservoirs. The best highlight of AM is that the large-area images provide a reference for selecting sites for further nano-micro structure analysis. The linkage procedure of AM images and FE-SEM facilitates the observation of the same nano-micron scale mineral or pore changes after different fluid actions. This technique is beneficial for studying the effect of fluid chemical reactivity transmission on reservoirs during reservoir development or CO2 geological storage. The mineral distribution phase diagram obtained by AM can be registered with the same position CT scan image, which can improve the accuracy of CT data to distinguish minerals. However, because AM itself is not good at identifying the fine types of clay minerals and because some mineral densities are similar, it increases the difficulty of CT image registration and segmentation, so the accuracy of the constructed 3D mineral distribution needs to be improved. With the improvement of the registration algorithm and in situ CT scanning accuracy, the combination of AM and CT will play a more important role in the study of the fluid reactive transport effect during reservoir development or CO2 geological storage, especially in the study of short-lived minerals and pore changes, as well as fluid migration.

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Investigation on dynamic propagation of fractures in shale induced by thermal fluid

Authors: Jiao Ge[1]; chuanjin yao[1]; qi zhang[1]; Baishuo Liu[1]; Fanyi Meng[1]; xingheng Huang[1]

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The connectivity of reservoir fractures is very important for the exploitation of shale oil resources. Shale reservoirs have extremely low permeability, and natural fractures are not developed, so it is not easy to form a complex fracture network. Therefore, it is generally solved by injecting into the rock to induce artificial fractures to improve the permeability of the formation. There are great differences in the micro-pores and micro-cracks evolution of shale reservoirs after high temperature convection heat, and the shale fracturing caused by high temperature is also obviously different in the mechanism. Not only does it change the mechanical mechanism of rock fracture, but also further affects the fracture morphology of shale reservoirs. The formation of fractures induced by high temperature thermal fluid is an excellent method to increase production, which can form a large scale fracture network in underground rock masses and improve production efficiency. Numerical simulation analysis of multiphysics coupling in porous media is the most economical and effective research method to solve many geological engineering problems at this stage. Based on the established thermo-hydro-mechanical coupling shale model, this study carried out numerical simulations on shale fracture propagation during high temperature thermal fluid injection. The research results show that the shale fracture propagation under the action of high temperature convection heat is the result of the combined action of hydraulic action and thermal stress. Thermal stress is the most dominant fracturing factor. The main fracture initiates at the wellbore and propagates along the direction of the maximum principal stress. The rock mechanical properties weaken, the fracture initiation pressure reduces, and the fracture propagation behavior becomes more complex.

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Poster / 698

Evaluating the performance of asphalt mixture with additives to withstand salt erosion and freeze-thaw cycles

Authors: Huining Xu[None]; Weidong Ji[None]

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Asphalt pavement is widely used in road construction due to its smoothness, wear resistance, and ease of maintenance, making it the most commonly chosen material. However, asphalt concrete exposed to the natural environment is susceptible to various external factors, resulting in different types and degrees of damage. This greatly shortens its service life and reduces the durability of asphalt pavement. Especially in coastal regions with seasonal freezing, salt spray, tides, and rainfall can all contribute to the penetration of salt into asphalt pavement through porous media. The inner salt will accumulate and dissolve, weakening the cohesiveness of the asphalt-aggregate interface and causing diseases such as spalling and pitting. In addition, the seasonal freeze-thaw cycle causes early damage to the asphalt mixture. Admixture is an effective means of improving the performance of porous asphalt mixtures. Efforts done by previous researchers have shown that ferrocyanide can inhibit salt crystallization and reduce salt erosion damage of porous materials. Basalt fiber and anti-stripping agent can improve the service performance of asphalt mixture. However, the effects of three additives on salt erosion and freeze-thaw coupling environments have not been studied, and their specific improvement effects are unclear.

This paper focuses on the damage resistance of asphalt mixture with crystallization inhibitor, basalt fiber and anti-spalling agent under salt erosion and freeze-thaw, respectively. The splitting tensile strength of asphalt mixtures with additives was tested after 15 cycles of salt erosion and freeze-thaw. We used X-ray computed tomography to analyze the initial internal structure after 0, 7, and 20 freeze-thaw cycles, as well as salt erosion. The effects of salt erosion and freeze-thaw cycles on asphalt mixtures with additives were evaluated through the analysis of changes in strength and internal structure. Based on the changes in internal structure, the performance enhancement of porous asphalt mixtures with additives was assessed using grey relation analysis and analytic hierarchy process analysis.

Results showed that the damage caused by salt spray erosion on the mechanical properties of asphalt mixture is greater than that of salt solution erosion. Compared to the AC-13 asphalt mixture, the SMA-13 asphalt mixture has better mechanical properties against the effects of freeze-thaw cycles and salt erosion. The performance improvement of asphalt mixture with a crystallization inhibitor is better than that of an anti-stripping agent and a basalt fiber asphalt mixture, respectively. The three types of additives only retard the evolution of internal structure and do not change the damaged formation of internal structure inside asphalt mixture under freeze-thaw cycles and salt erosion. The internal damage index of asphalt mixture with crystallization inhibitor is the minimum, indicating good resistance to freeze-thaw cycles and salt erosion. The combination of SMA-13 gradation and crystallization inhibitor was found to be suitable for designing asphalt mixtures in coastal seasonal frozen regions. The research results will help improve the level of construction and maintenance of asphalt pavement in coastal seasonal freezing areas, extend its service life, and save on maintenance costs.

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Experimental investigation on phase behavior of pyrolysis hy-

drocarbon products from Chang 73 medium-low maturity shale

Authors: Baishuo Liu[1]; Chuanjin Yao[None]; Fanyi Meng[2]; 楠陈[None]; 慧超杨[None]; Xin'ge Du[None]

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Low-to-medium maturity shale oil reservoir is an important unconventional energy source with small pore size and poor fluid flow ability. In-situ pyrolysis is one of the effective methods for developing low-to-medium maturity shale oil reservoirs. On the one hand, the pyrolysis of organic matter in low-to-medium maturity shale produces complex fluids, mainly including pyrolysis oil and pyrolysis gas. On the other hand, the fluid generated after pyrolysis begins to migrate due to thermal expansion, thereby promoting the effective development of low-to-medium maturity shale reservoirs. It is worth noting that the composition of pyrolysis fluid products can change with changes in heating temperature and heating time. The changes in fluid compositions in porous media can lead to changes in their phase behavior characteristics, and accurately characterizing pyrolysis fluid phase behavior is of great significance for predicting oil and gas production in reservoirs. In the paper, the Chang 73 medium-low maturity shale were selected and ground into particles, a pyrolysis experimental device for low-to-medium maturity shale was constructed, and pyrolysis experiments were conducted on shale particles at different temperatures. Gas chromatography and mass spectrometry techniques were used to analyze the composition of fluid products under different pyrolysis conditions. In addition, an experimental device for studying pyrolysis fluid phase behavior characteristics was constructed, which increased the maximum experimental temperature to 300℃ compared to existing devices. The experimental data can be obtained is more extensive and can better reflect actual oilfield conditions. Constant mass expansion experiments were conducted on pyrolysis fluid products at six temperatures (20-300℃) to observe the characteristics of oil gas interface changes under different temperature and pressure conditions. The experimental data were fitted and the fluid bubble point pressure at different temperatures was obtained. The P-T (pressure-temperature) phase diagrams were drawn and compared with the calculated results of the PR (Peng-Robinson) equation, the PR equation is the main method for describing fluid phase behavior in numerical simulations. The results showed that as the pyrolysis temperature increased, the lighter component of C3-C12 in the pyrolysis oil increased, and the C3-C7 had the highest content at 425℃. The content of C1 and C2 in the pyrolysis gas increased with the increase of temperature. Under the condition of 425℃, the bubble point pressure of pyrolysis fluid products first increases and then decreases with temperature. The P-T phase diagram obtained from the experiments has the same trend as the calculated phase diagram from PR equation, but there is also a significant difference. This indicates that correcting the PR equation is of great significance, as it is the key to accurately characterize the phase behavior characteristics of pyrolysis products of low-to-medium maturity shale.

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MS03 / **700**

Quantifying the effect of matrix diffusion on tracer transport in fractured reservoirs

Author: Hui Wu[1]

Co-author: Yuanyuan Wei [1]

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Tracer testing is commonly used to characterize fracture flow and transport processes. The interpretation of tracer data requires numerous forward simulations of tracer transport in a 3D fracture-matrix model, leading to significant computational burden. As matrix permeability is generally several magnitudes smaller than fracture permeability, some studies only considered a 2D fracture model to alleviate the computational burden. However, the impact of matrix diffusion, a mechanism that may affect tracer transport even in an extremely low matrix permeability model, is unclear. This study quantitatively investigates the effects of matrix diffusion on tracer transport through an analytical solution. Based on the results, we discuss the situations in which matrix diffusion has minimal effect on tracer transport and therefore matrix can be safely ignored. A dimensionless number that integrates fracture/matrix parameters and injection parameters is proposed to estimate matrix diffusion effect on tracer transport. For situations that matrix diffusion can not be ignored, we develop an equivalent injection function to accurately quantify the effect of matrix diffusion in a 2D fracture (matrix-free) model. The feasibility of the dimensionless number as well as the equivalent injection function is further examined through numerical simulations which consider complex geological conditions.

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MS06-B / **701**

Numerical modeling of the phase separation process driven by a porous membrane

Authors: Mengyi Jiang[1]; Guang Yang[None]; Jingyi Wu[1]

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The separation of liquid and gas phases using porous media has been considered for various applications such as propellent management in aerospace, petroleum engineering, carbon storage and so on. However, such a process is usually difficult to model as the multiphase flow involving porous media usually spans several characteristic lengths, and the interface conditions between the free fluid and the porous media flow are relatively complex. A direct numerical simulation (DNS) using fully resolved Navier-Stokes equations is limited by the immense computational cost. In this work, a mixed-dimensional flow model was developed for the highly coupled free fluid and thin porous media flow, in which the flow process in the porous membrane was reduced to one dimension. Besides, the parameter transfer equations at the regional interface were evaluated, and the proposed model was validated against DNS results. The effects of pore structures, porosity, and flow direction on the two-phase transport process were studied in detail. The present study will provide guidance for the optimization of phase separation systems driven by thin porous media.

Keywords: phase separation, multiphase flow, numerical modeling, coupled flow, porous media

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Quantitative investigation on distribution characteristics of organic matter in medium-low maturity shale and its pyrolysis products after in-situ conversion by NMR

Authors: Chuanjin Yao[None]; Baishuo Liu[1]; Jiao Ge[1]; Yaqian Liu[2]; Yangyang Xuan[None]; Jingxuan Hou[None]

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Low-to-medium maturity shale oil reservoirs are widely distributed in China and have received widespread attention from domestic and foreign researchers in recent years. In-situ pyrolysis conversion is one of the main methods for developing low-to- medium maturity shale oil reservoirs. In the process of pyrolysis, on the one hand, rock minerals expand due to heat, and on the other hand, the organic matter inside the shale continuously pyrolysis to produce oil and gas, which expand and flow due to heat. The two effects lead to continuous changes in the distribution space of pyrolysis fluids of low-to-medium maturity shale. Clarifying the distribution characteristics of organic matter

and its pyrolysis products after in-situ conversion is of great significance for clarifying the development mechanism of low-to-medium maturity shale oil reservoirs. In recent years, nuclear magnetic resonance (NMR) technology has received widespread attention as a method for analyzing the distribution of fluids in porous media. The technology can reflect the fluid distribution in pore spaces of different sizes by analyzing the intensity of hydrogen signals at different relaxation times. In the paper, low-to-medium maturity shale samples from Chang 73 block were selected and cut into cores. A pyrolysis experimental device for low-to-medium maturity shale was independently designed and constructed. Pyrolysis experiments were conducted on the shale cores under different temperature conditions, and NMR testing was conducted on the shale cores before and after pyrolysis to clarify the pore structure characteristics of non-pyrolysis shale and the main storage space of organic matter. After pyrolysis, the shale cores were saturated with white oil, and based on the NMR results after pyrolysis, the main storage space of pyrolysis organic matter was determined. In addition, the density and porosity pyrolysis variation characteristics of the shale core were also clarified based on the quality difference method. The results show that the shale core underwent significant deformation and expansion after pyrolysis, and a large number of fractures were generated. The organic matter was mainly concentrated in the pore space corresponding to relaxation time of 0.1ms, and the pore space of the shale core significantly increases after pyrolysis. The pore space of the shale core is the largest at the final temperature of 400℃, and the pyrolysis oil was mainly distributed in the pore space with a relaxation time of 100-1000 ms.

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MS09 / 704

Digital Porous Material Analysis with Multiscale REV

Author: Julien Maes[1]

Co-authors: Hannah Menke [2]; Yong Wen-Pin [3]; Dmytro Petrovskyy ; Kamaljit Singh [1]

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Digital Porous Media Analysis (DPMA) is the process of using imaging and simulation techniques (e.g., x-ray computed microtomography, Pore-Network Modelling (PNM) and Direct Numerical Simulations (DNS)) to investigate the properties of porous materials. With DPMA, physical processes are investigated in the real structure of a sample and effective porous media properties (e.g., permeability and capillary pressure) are estimated. These properties can then be used for upscaling,

provided that the sample investigated is a Representative Elementary Volume (REV) of the full domain of interest. However, most porous materials relevant to the energy transition are multiscale, and thus have pore structures (e.g., microporosity, channels, vugs) spanning several orders of magnitude in size. An REV of such materials cannot be fully characterised by a single image, which would either be too small to be an REV or lack the resolution to accurately resolve the pore/solid interfaces. In this work, we define a multiscale REV of a porous material as an image that can be segmented into resolved and unresolved parts, and for which, for each unresolved voxel, the properties can be associated with a higher resolution image that is an REV of the underlying structure inside that voxel, the combination of which provides an REV of the full domain of interest. Our multi-scale REV workflow is demonstrated on several examples, including microporous carbonate rocks and 3D printed hierarchical foams, and employs multiscale simulation techniques (e.g., Darcy-Brinkman-Stokes models, multiscale PNM) first to confirm a multi-scale REV and then to simulate reactive transport and multiphase flow processes while estimating properties such as permeability, dispersivity and capillary pressure.

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MS16 / 705

Color Properties and Porous Ink Layer –a study via Optical Spectroscopy

Author: Nicolae Tomozeiu[1]

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The world of printing is rapidly and extensively developing due to the progress made in the inkjet technology. This printing technology delivers good print quality using the flexibility of digital printing at a breakthrough cost price. The R&D department of Canon Production Printing company, is a major player in the development of inkjet technologies for many different applications.

The physical processes which regulate the interactions between ink droplets and a thin porous paper have been the subject of many studies considering both theoretical understanding and sustainable industrial applications.

Understanding the processes as ink spreading, evaporation and imbibition into porous material is vital for having prints of high quality. Experimental studies based on Optical Spectroscopy & Microscopy, Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance (NMR), Automatic Scanning Absorptometer (ASA), etc have been used to get in-depth of these physical phenomena, which design the print drying. The result of drying process is an ink solid thin film formed onto porous paper. We have to consider a surface topography of the ink layer, as well as a resulted interface ink/paper. Due to the complex drying process, the ink layer might have a (in)homogeneous

distribution of the pigment particles into the polymeric matrix. Also, our SEM studies showed the presence of the voids of various dimensions into this structure.

The outputs of a print process are image quality and print robustness. This means optical and mechanical properties of the thin ink layer onto porous paper. In this work, VIS optical spectroscopy is employed on both the computational simulation (Scout code program) and the experimental studies to reveal the relation between the compositional properties (pigment distribution, layer thickness, concentration and distribution of voids) of the ink layer and the color properties of the print.

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Poster / 708

Optical Properties versus Compositional & Structural Features of Dried Ink Thin Films

Authors: Hamid Mansouri[1]; Helder Marques Salvador[1]; Nicolae Tomozeiu[2]

[1] *R&D Depart. Canon Production Printing B.V.*

[2] *Canon Production Printing B.V.*

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The water-based inks with polymeric latex particles used in printing technology deliver prints of superior quality at a low cost and environmental friendly. Via ink formulation and drying processes, the inkjet prints are characterized by a wide color gamut, intense gloss with tonal graduations and excellent mechanical properties.

Our study delves into enhancing the optical performance of these inks and printing processes by examining how light interacts with the printed porous surface. The ink's composition features pigments and polymeric beads randomly dispersed with interparticle spaces or fissures. Utilizing High-Resolution SEM imaging, we scrutinize the structure and local makeup of the ink layers post-printing, while VIS spectroscopy aids in assessing their optical attributes.

We employed ray tracing to construct an optical model for colored prints, aiming to forecast the reflected optical spectrum from prints possessing specific porous structures, determined by the spatial arrangement of latex, pigments, and voids/cracks. To ensure accuracy, the model's parameters align with those of a VIS spectrophotometer, maintaining consistent light spectra and angles.

Our results demonstrate the reliability of ray tracing, validated by experimental data, particularly for monochromatic layers on coated substrates. By integrating the print's structure and the optical characteristics of its constituents, we achieved a harmonious match between empirical and modeled outcomes.

Concluding our research, we conducted sensitivity analyses on color coordinates (L, *a*, b*), examining variables like layer thickness, pigment concentration, coverage, and ray count. This exploration offers insights into the intricate interplay between light and porous ink layers, advancing our understanding of their optical behavior.

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709

Experimental investigation on fluid flow characteristics in shale reservoirs with different types of fractures

Authors: Huichao Yang[None]; Chuanjin Yao[None]; Zhe Wang[None]; Baishuo Liu[1]; Jiawei Zhu[None]; Lei Li[None]

[1] 中国石油大学（华东）

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Energy security is very important to the development of the country. With the gradual reduction of conventional oil and gas resources, unconventional oil and gas resources represented by shale oil and gas have gradually become the focus of exploration and development, and have broad prospects for development. Gas injection and horizontal well volume fracturing technology are commonly used to extract shale oil at home and abroad. However, the understanding of the fluid flow mechanism of multi-scale pore-fracture system under the condition of multi-stage fracturing of horizontal wells in shale reservoirs is still unclear at present. It is necessary to systematically and deeply study the fracture flow characteristics of shale reservoirs, and to clarify the influence of different fracture types and fracture parameters on the fluid flow law in shale reservoirs, so as to provide theoretical support for the actual development of the field. Therefore, this article processed simulated natural fractured rock cores with different fracture openings and fracture densities through wire cutting and placement of metal gaskets. Fluid flow experiments were conducted under different displacement pressure differentials, and fluid flow patterns within natural fractures in shale oil reservoirs were summarized and analyzed. The results show that due to the influence of gas sliding effect, the gas permeability of the core in the low-pressure range is significantly higher than that under the high-pressure condition. There are nonlinear and linear segments in the low-speed flow of liquid in natural fractures, and the nonlinear characteristics decrease with the increase of fracture opening and fracture density, and increase with the increase of fluid viscosity. Compared with the simulation of natural fractures, the presence of quartz sand proppant in simulated artificial fractures significantly improves the conductivity of the core. The liquid flow pattern conforms to the seepage of high-permeability porous media, and the relationship between formation water and crude oil flow conforms to the linear formula.

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MS17 / 710

Effect of pH on the Competitive Adsorption Behavior of CO2/CH4 in Shale Inorganic Nanopores from the Molecular Simulations

Author: Shaofeng Ning[1]

Co-authors: Jingkai Cui [2]; Junyao Bao [2]; Shiyuan Zhan [2]; Xiaoguang Wang [1]

[1] *Chengdu University of Technology*

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Objectives/Scope:
Geological Carbon Storage (GCS) in depleted tight reservoirs is considered a promising technology for reducing carbon dioxide emissions. These tight reservoirs feature numerous nanoscale pores that provide ample adsorption space for gases. However, the pH values of the reservoir pores vary, and the extended exposure to different pH environments over time can result in distinct surface properties of inorganic nanopores on quartz (pH effects characterized by the deprotonation degree of silanol groups on the quartz surface). This variability may impact the adsorption capacity of gases, but the mechanisms remain unclear. Therefore, a comprehensive understanding of gas adsorption mechanisms, considering reservoir pH values, is crucial for CO2 sequestration and enhancing methane recovery rates (EGR). This study employs GCMC simulations to investigate the competitive adsorption mechanisms of CO2/CH4 in shale inorganic nanopores on quartz, taking into account reservoir pH conditions.
Methods/Procedures/Process:
*The adsorption of CO2, CH4, and a CO2:CH4=1:1 mixture was investigated at reservoir conditions of 353.15K and pressures up to 50MPa. The pH conditions ranged from 2-5, 5-7, to 7-9, corresponding to deprotonation degrees of 0%, 9%, and 18%, respectively. Quartz nanopores, CH4, and CO2 were modeled using the CLAFF, TraPPE-UA, and TraPPE-EH models. GCMC simulations were conducted using the MCCCS Towhee software. Each simulation consisted of 2×108 steps in total, with 5×107 steps for equilibration and 1.5×108 steps for statistical sampling. Atomic trajectories were saved every 2000 steps for subsequent data analysis. Using the simulated results, we computed the one-dimensional and two-dimensional density distributions of gases, as well as the excess adsorption. Additionally, we accounted for changes in adsorption phase volumes under three pH environments to calculate the absolute adsorption amounts.*Results/Observations/Conclusions:
The study revealed that with an increase in deprotonation degree, the adsorption phase volumes of CO2 and CH4 slightly increased in both single-component and competitive adsorption scenarios. In competitive adsorption, the injection of CO2 exhibited a more pronounced effect in reducing the adsorption density of CH4 as the deprotonation degree increased（corresponding increase in pH） In

single-component adsorption, both the excess adsorption and absolute adsorption of CO2 increased with the increasing deprotonation degree, while the impact on CH4 was minimal. In competitive adsorption, CO2 significantly decreased the excess adsorption of CH4, and beyond a pressure of 30MPa, the excess adsorption even became negative. With an increase in deprotonation degree, both the excess adsorption and absolute adsorption of CO2 increased, while the adsorption of CH4 slightly decreased. This suggests an enhancement in the competitive adsorption capability of CO2.
*Applications/Significance/Novelty:
This study provides molecular-level insights into the adsorption behavior of CO2/CH4 in quartz nanopores under varying pH conditions. The findings contribute to establishing a theoretical foundation for CO2 storage and methane recovery enhancement under reservoir conditions with different pH levels.

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References:

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712

Quantitative characterization on forced imbibition characteristics of shale oil reservoirs based on nuclear magnetic resonance method

Authors: Chuanjin Yao[None]; Huichao Yang[None]; Xinge Du[None]; Baishuo Liu[1]; Jiawei Zhu[None]; Hailong Zhao[None]

[1] 中国石油大学（华东）

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The development of shale reservoirs has gradually become the focus of global energy attention, and large-scale volume fracturing of horizontal wells has become a cost-effective means of developing shale reservoirs. After large-scale fracturing of different types of shale reservoirs, the fracturing fluid will produce strong imbibition effect in the reservoir, resulting in low flowback rate of fracturing fluid. There are problems such as pressure change, unclear understanding of oil production law and unknown influencing factors in the forced imbibition stage. In this paper, aiming at the main shale oil reservoirs in China, the cores of some blocks in Qinghai and Gulong areas are selected. Combined with the actual conditions of reservoir reservoirs, the study on the forced imbibition law of different types of shale oil is carried out. Combined with nuclear magnetic resonance technology, the characteristics of forced imbibition and the differences in the microscopic production law of crude oil are clarified, and the influence of core permeability and contact angle on forced imbibition is further analyzed. The results show that the shale has a strong imbibition effect on the fracturing fluid, the oil phase content in the core decreases, and the oil-water replacement phenomenon occurs. There are preferential pores in the fracturing fluid during the imbibition process, and the fracturing fluid preferentially enters the smaller pores, and can cause a short-term increase in the oil phase content in the larger pores. With the continuous process of imbibition, the rate of imbibition oil gradually slowed down, and the fracturing fluid gradually infiltrated into the rock sample. Both permeability and wettability can affect the imbibition ability of fracturing fluid. For rock samples with similar properties in the same area, the higher the permeability and the smaller the contact angle, the less the oil phase content after imbibition, and the more obvious the imbibition effect of fracturing fluid.

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MS03 / **713**

Fracture-matrix interaction, fluid flow and chemical movement in low-permeability fractured media

Author: Qinhong Hu[1]

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

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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 fractures into the 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 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). This work discusses various, and complementary, approaches to investigating pore structure, and the resulting anomalous imbibition and diffusion, in low-permeability Yucca Mountain welded tuff of Nevada, as well as various shales of USA and China undergoing active exploration and production. Using an innovative and complementary laboratory approaches, such as imbibition and diffusion tests employing a recipe with several nano-sized tracers and subsequent microscale mapping on the shale, our work indicates the limited fracture–matrix interactions in fractured shale, with low pore connectivity of predominantly nm-sized shale matrix pores and the consequent limited (sub-mm near the fracture face under atmospheric pressure and temperature) accessible porosity and anomalous diffusion to the stimulated fracture network and producing wellbore. The presentation will end with some ongoing work of coupled thermal-hydraulics-mechanical-chemical tests and gas-liquid flooding experiments of low-permeability media with lamina.

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MS13 / **714**

Quantifying oil- and water-wettable pore networks of the lacustrine- and marine-sourced shale oil reservoirs

Authors: Qinhong Hu[1]; Yuxiang Zhang[None]; Cunjian Zhang[None]; Tao Zhang[None]; Qiming Wang[None]; Yubin Ke[None]; He Cheng[None]; Xiuhong Li[None]

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

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Microscopic pore structure (both geometry and connectivity) characteristics control fluid flow and hydrocarbon movement in shale oil reservoirs. Considering the uniquely wide spectrum of pore sizes (nm to sub-mm), microscale mixed wettability, as well as the interplay of pore structure and wettability in organic-rich shale oil reservoirs, this work presents various approaches to quantifying the oil- and water-wettable pore networks for several important tight oil formations in China and USA with different depositions, as well as a range of maturation and mineral compositions. The approaches include the utility of different wetting fluids (deionized water or API brine, n-decane and/or toluene, isopropyl alcohol or tetrahydrofuran or dimethylformamide), fluid pycnometry, fluid immersion porosimetry after vacuum saturation, mercury intrusion porosimetry, nuclear magnetic resonance, and field emission-scanning electron microscopy. In particular, (ultra-) small angle neutron & X-ray scattering techniques, (U)SANS & (U)SAXS, are used to quantify the total (both edge-accessible and isolated) porosity and characterize pore size distribution in a pore length size from 1 nm to 10 □m; in addition, the employment of contrast matching technique of (U)SANS enables the

discrimination of accessible (open) pores and inaccessible (closed) pores to a particular liquid fluid. For example, our results show that the marine-sourced Bakken samples in USA have a relatively high total porosity (8.87-12.95%) with no more than 30% of the pores are accessible from sample surface, and are not preferentially wet by oil or water.

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MS06-A / 715

A comprehensive analysis on the wettability in shale oil rocks

Authors: Xiao Wenlian[1]; Yubin Yang[1]; jitian Ren[1]

Co-authors: Chu Huang [1]; Hui Tang [1]; Lingli Zheng [1]; Qihong Lei [2]; Suwei Ma [2]; Wanfen Pu [1]; Youan He [2]

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

[2] *PetroChina Changqing Oilfield Company*

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Abstract: Fracturing-Soaking-Producing (FSP) is considered one of the effective methods in the development of shale oil. Improving the imbibition efficiency during the FSP process cannot be achieved without accurate understanding of reservoir wettability. Here, we used contact angle wettability method, spontaneous imbibition wettability method with nuclear magnetic resonance, centrifugation wettability method, and freeze-emission electron microscopy method to evaluate the wettability of core samples withdrew from Ordos Basin. At the same time, we developed a characterization method for pore-scale wettability based on the capillary bundle model then quantified the pore-scale wettability characteristics. The freeze-emission electron microscopy experimental results behaved that the oil is mainly adsorbed on the pore surface, while the water is present as a free fluid in the pores. The capillary pressure curves during waterflooding agree with the ones during gasflooding, and the wettability index is between 0.55 and 0.65, indicating that our core samples exhibit oil-wet. Furthermore, the pore-scale wettability illustrated that the average proportion of oil wet pores is about 60%, and the average proportion of water wet pores is about 40%. The oil-wet pores are mainly distributed in mesopores, and the micropores and macropores account for a relatively small proportion. The water-wet pores are mainly distributed in macropores and micropores, and the mesopores account for a relatively low proportion. Our research work enriches the understanding of the wettability of shale oil and has certain significance for optimizing the parameters such as the amount of liquid entering the shale oil reservoir.
Keywords: shale oil; wettability; pore structure; pore scale

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MS17 / 717

A three-dimensional reservoir-scale Thermal-Hydrological-Mechanical model of enhanced geothermal systems

Author: Tingting Liu[1]

Co-author: Hang Deng [1]

[1] *Department of Energy & Resources Engineering, Peking University*

Corresponding Authors: hangdeng310@gmail.com, tingting.liu@pku.edu.cn

The heat energy resource in the deep earth (3 ~10 km), which is carried by Hot Dry Rocks (HDR), has a huge capacity for geothermal power generation. As a type of conductive geothermal energy, HDR has low rock permeability, so that Enhanced/Engineered Geothermal System (EGS) is developed to artificially increase the heat exchange area and further extract the deep geothermal energy with the connected natural fractures and hydraulic stimulated fracture network. The coupled Thermal-Hydrological-Mechanical (THM) processes largely control the heat recovery efficiency from HDR, and thus real 3D reservoir scale investigations that account for the multiphysics coupling mechanisms are needed to inform geothermal energy recovery from HDR.

In this work, we built a three-dimensional THM model for the EGS of Qiabuqia HDR (Zhang et al. 2018, Gonghe Basin, China) by taking advantage of the novel simulation framework, GEOSX (Settgast et al. 2022). As a rapidly growing open-source multi-physics simulator, GEOSX has highly scalable algorithms for solving complex fluid flow, thermal, and geomechanical coupled systems. Preliminary geological data of the target area has been acquired by exploratory wells (e.g., GR1, GR2, DR3, DR4). There is also a trial production well GH-01. In our model, we considered a dual-well utilization system. Our 3D model focuses on reservoir-scale THM coupling, and takes into consideration the geostress directions in configuring the faults and (hydraulic)fractures, which are explicitly handled with EDFM (Embedded Discrete Fracture Model) method. The simulated results of heat recovery efficiency under different production scenarios provide guidance information for engineering practices.

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R. Settgast, C. Sherman, B. Corbett, S. Klevtsov, Francois Hamon, A. Mazuyer, A. Vargas, TotoGaz, N. Castelletto, M. Cremon, M. Cusini, J. White, B. Han, Hmmorgan, J. Huang, Y. Hao, Herve Gross, W. R. Tobin, Sy-Tuan Nguyen, A. Franceschini, X. Lacoste, M. Yoder, Robinspb, M. N'diaye, Shabnamjs, A. Borio, Labesse40, Robinson96, M. Khait, and S. Fram- bati. Geosx/geosx: v0.2.1-alpha, 2022. URL https://zenodo.org/record/7151032. S. Zhang, Y. Weide, L. Dunpeng, J. Xiaofeng, Z. Shengsheng, L. Shengtao, F. Lei, W. Haidong, Z. Zhaofa, L. Zhiwei, M. Jianqiang, C. Zhengpu, and H. Lisha. Characteristics of geothermal geology of the qiabuqia hdr in gonghe basin, qinghai province. GEOLOGY IN CHINA, 45 (6):1087–1102, 2018.

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Poster / 718

Promoting Ultra-High-Density Nanoparticles Exsolution in Layered Perovskite Ferrites via a Facile Cobalt Doping Method: A High-Performance, Stable Anode for Direct Ethane Solid Oxide Fuel Cells

Author: Rubao Zhao[1]

Co-author: Shuo Zhai [1]

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Nanoparticles anchored on the perovskite surface have gained considerable attention for their wide-ranging applications in heterogeneous catalysis and energy conversion due to their robust and integrated structural configuration. Herein, we employ controlled Co doping to effectively enhance the nanoparticle exsolution process in layered perovskite ferrites materials. CoFe alloy nanoparticles with ultra-high-density are exsolved on the (PrBa)0.95(Fe0.8Co0.1Nb0.1)2O5+δ (PBFCN0.1) surface under reducing atmosphere, providing significant amounts of reaction sites and good durability for hydrocarbon catalysis. The morphology evolution measurements reveal a significant transform in CoFe alloy nanoparticles at around 600 ℃, transforming from larger to ultra-densely decorated smaller nanoparticles. A single cell with PBFCN0.1 anode exhibits high performance in wet ethane atmosphere (e.g., a typical peak power density of 455 mW cm−2 at 800 ℃), which is significantly improved by 36%-70% compared to the sample without Co doping. This discovery emphasizes how temperature influences alloy nanoparticles exsolution within doped layered perovskite ferrites materials, paving the way for more targeted material-specific research and broadening the spectrum of practical applications.

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MS01 / **720**

Feasibility of injecting CO2 into low-permeability gas reservoirs to enhance gas recovery

Author: Ermeng Zhao[1]

[1] *Peking University*

Corresponding Author: zhaoermengnepu@163.com

Natural gas resources in tight sandstone are huge, but the gas production rate decreases rapidly and the gas recovery rate is low due to poor reservoir physical properties. Injecting CO2 when the gas reservoir is depleted can enhance gas recovery and simultaneously sequestering a large amount of greenhouse gases, which has significant economic and environmental benefits. To fully understand the production mechanism of the CO2 flooding process at the field scale and evaluate the technical feasibility, a mathematical model is established to study the dynamic behavior of the method in this work. Based on the geological data of the Sulige gas field in the Ordos Basin, a 3D numerical simulation model of CO2 flooding in tight gas reservoirs under the five-point well pattern is established. The production dynamic behavior of enhanced gas recovery and CO2 storage processes is studied through numerical simulation approach. Moreover, the impact of engineering and geological parameters on production performance is discussed, such as perforation strategy, CO2 injection rate, permeability, porosity, diffusion coefficient, residual water saturation, reservoir thickness, etc.

Results indicate that the CH4 production rate is significantly increased after CO2 flooding, and the gas recovery can be increased by up to 19.2%, confirming the feasibility of CO2 injection technology to enhance CH4 production in depleted tight gas reservoirs. According to the spatial distribution characteristics of the components, the reservoir can be divided into CO2 zone, CH4-CO2 mixed zone, and CH4 zone. Although a CO2-CH4 mixing zone is formed due to diffusion, there was no significant mixing in the reservoir, ensuring the purity of natural gas in the production wells. Once the CO2 breakthrough occurs, the CH4 production rate decreases rapidly, and the spatial distribution of CO2 is only slightly affected by the gravity difference of the components. These characteristics are significantly different from those of high-permeability gas reservoirs. The CO2 front in the early stage of flooding is proportional to the square root or cube root of time, depending on the perforation location and reservoir thickness. However, the CO2 front in the late flood stage shows a linear relationship with the square of time. It is recommended that injection well and production well be fully perforated in the gas interval because the enhanced gas recovery is higher than other perforation options and excessive bottom-hole pressure in the injection well can be avoided. As the permeability increases, the CO2 breakthrough time becomes shorter, and the CH4 recovery increases, resulting in less CO2 buried in the reservoir. The diffusion coefficient has a significant impact on production dynamics. The larger the diffusion coefficient, the wider the mixing range of CH4 and CO2, which accelerates the CO2 breakthrough and leads to low CH4 recovery.

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Poster / 725

Comparative verification of hydro-mechanical fracture behavior: Task G of international research project DECOVALEX–2023

Authors: Mostafa Mollaali[None]; Wenqing Wang[1]; Keita Yoshioka[2]; Olaf Kolditz[3]

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Numerical simulations become necessary when experimental approaches cannot cover the required physical and time scale of interest. One such area is a simulation of long-term host rock behaviors for nuclear waste disposal and simulation tools involved in the assessment must go through rigorous validation tests. The DECOVALEX project (Development of COupled models and their VAlidation against EXperiments) is dedicated to this purpose by international participants\footnote{www.decovalex.org}. This work is part of the ongoing phase DECOVALEX–2023 (D–2023, Task G) particularly aiming to simulate fracture behaviors under various conditions. Here, we cross-verified a variety of numerical methods including continuous and discontinuous approaches against four benchmark exercises with emphasis on numerical accuracy and parameterization of the various numerical approaches. The systematic inter-comparisons of test cases highlight the advantages and disadvantages of the different numerical models. Numerical details on discretization effects (e.g. mesh density and orientation) and domain size were investigated in detail for practical applications. It became evident that meticulous attention to mesh resolution and domain size is imperative for achieving accurate numerical simulations, even for static cracks. Moreover, when comparing numerical methods to closed-form solutions for static cracks, all models successfully reproduced the maximum crack opening but encountered challenges near the crack tips. Finally, the paper discusses how to convert between and therefore compare parameters of various numerical approaches. Our benchmark studies reveal that each model necessitates a distinct number of parameters, even in simple scenarios like static crack aperture benchmarks. It is generally more practical to employ fewer parameters to mitigate model over-parameterization and enhance experimental feasibility.

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MS01 / **727**

Microfluidic Study of Formation, Dissociation, and Dissolution Dynamics of Gas Hydrates in Porous Media

Author: Wei Yu[1]

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Gas hydrates are crystalline solids in which guest molecules are trapped within cages formed by water molecules at high pressure and low temperature. These solids have important applications in natural gas hydrate exploration, CO2 or H2 storage, water desalination, gas separation, and gas/oil transportation. Natural methane (CH4) hydrates are abundant in the seabed sediments and are potential sources for future energy harvesting1. On the other hand, carbon dioxide (CO2) hydrates are promising forms of CO2 sequestration due to the large storage capacity. The phase transition of hydrates and the transport behaviors of the relevant gas and liquid phases in porous media are crucial to CH4 production and CO2 storage using hydrates. Therefore, many studies have been conducted on investigating the dynamics of formation, and dissociation of CH4 and CO2 hydrates in porous media using sand or glass bead packs with the help of in-situ imaging methods such as X-ray synchrotron tomography and magnetic resonance imaging (MRI) technology. In this work, we developed a low-temperature and high-pressure microfluidic system for gas hydrate study, allowing for in-situ imaging of the phase transition of hydrates under realistic reservoir conditions of deep seabeds. We studied the formation, dissociation, and dissolution mechanisms of CH4 and CO2 hydrates in both pore scale and chip scale. The hydrates were generated in pure water at 10 MPa and 5 oC subcooling temperature. The dissociation of these two hydrates was induced by decreasing pressure and increasing temperature, respectively. During hydrate formation, we observed the nucleation and propagation of hydrates from the gas-liquid interfaces into the bulk gas, showing various morphologies at the pore scale. The growing kinetics were calculated by analyzing the optical images obtained by a high-resolution camera. Further, we successfully captured the crustal fingering of CH4 gas encased by CH4 hydrates due to the local pressure gradient 2. From the chip scale, the location of hydrate formation and its propagation in the porous media is stochastic. We found that the induction time for hydrate formation is also stochastic, and the nucleation of hydrate should be triggered by external stimuli such as flow and pressure[3]. During hydrate dissociation, the hydrates remained stable until the pressure or temperature exceeded equilibrium. Then, a drastic transition of hydrates into gases occurs, which results in the fast displacement of gas with liquid in the porous media. In addition, the reformation of hydrates was observed during hydrate dissociation. Finally, we studied the dissolution of CH4 hydrate in undersaturated water and revealed the formation, dissolution, exsolution, and reformation mechanisms of gas hydrates in porous media.

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1 R. Boswell and T. S. Collett, "Current perspectives on gas hydrate resources,"Energy and Environmental Science, vol. 4, no. 4. pp. 1206–1215, Apr. 2011. doi: 10.1039/c0ee00203h. 2 Xiaojing Fu et al.,

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Conference Proceedings:

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Poster / **728**

Reactivity of porous media under continuous injection

Author: Dario Maggiolo[1]

Co-author: Angela Sasic Kalagasidis [1]

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High flow rates within reactive porous media occur both in industrial applications and in natural media, e.g. in permeable soil substrates subjected to extreme weather events [1,2]. The reactive surfaces of the soil grains interact with the transported species, determining the overall porous media reactivity and capacity of retaining nutrient and contaminants. We show via pore-scale lattice-Boltzmann simulations in a packed bed column that, under the conditions of uniform injection, the uniformity of porous surface reactions is determined by the mixing of the low concentration wakes forming behind the reactive soil grains. Scaling arguments are proposed to extract analytical models for the probability distributions of concentrations at the reactive surfaces.

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References:

1 Pettersson, Kaj, et al. Journal of Hydrology 603 (2021): 126851. 2 Maggiolo, Dario, et al. Physical Review Fluids 8.2 (2023): 024502.

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MS05 / **729**

Exploiting induced carbonate precipitation to improve reservoir storage integrity and geothermal system efficiency

Author: Philip Salter[1]

Co-authors: James Minto [1]; Jay Warnett [2]; Katherine Dobson [1]

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Biomineralization, through microbially, thermally, or enzyme induced carbonate precipitation (MICP/TICP/EICP), is a cost-effective cementation process for changing porosity and permeability in the subsurface. This study aims to optimize compositional and injection parameters for biomineralization fluids, and to develop understanding of the interactions between geochemical reactions and fluid transport properties at the pore (micron) scale. Utilizing real-time in situ X-ray computed tomography (XCT), we compare traditional Microbially Induced Calcium Carbonate Precipitation (MICP) with novel thermally delayed (TICP) and Enzyme Induced Calcium Carbonate Precipitation (EICP) in a range of lithologies. This allows us to investigate the impact of mineralogy, grain size distribution, and temperature as well as the injection composition and strategy. We present quantitative analysis of crystal locations, the volume of carbonate and of individual crystals, and the effect of crystals on permeability and flow localisation over time. Coupled to measured changes in microstructural and macroscopic properties over repeated precipitation and dissolution cycles we present refined models of reactive transport for different injection strategies, and identify the optimal treatment strategy for different subsurface applications. This includes validation of the durability of precipitated calcite during dissolution phase simulating the behaviour of CO2-enriched brines.

This work provides the underpinning understanding principles of crystal formation, growth and hydrodynamic feedback mechanisms necessary for accurate modelling of reservoir scale dynamic processes. However we also show how TICP and EICP strategies can improve performance of real-world Carbon Capture and Storage systems, driving more homogeneous, widely distributed and larger volumes of precipitated CaCO3 by maintaining permeability during treatment at higher degrees of cementation when compared to MICP. We also show how variable injection strategies allow improvement of other physical properties (e.g. mechanical strength) and enables the addition of highly conductive additives or phase change materials without reducing precipitation and flow. Using CaCO3 precipitation we observed a 470% increase in the thermal conductivity of unsaturated quartz sand after 9 cycles of MICP, and an 800% increase following addition of 5 wt% expanded natural graphite (ENG). Our findings also demonstrate the compatibility of integrating paraffin as a phase-change material within the porous structure of ENG prior to MICP/EICP treatment significantly increasing specific heat capacity. These new geomaterials have widespread implications for thermal energy storage, specialized geothermal grouts/backfill, shallower wells and reduced geothermal energy costs.

The project's outcomes impact the commercialization of engineered biomineralization and its role in the subsurface energy transition.

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Poster / 730

The effect of fractures and heterogeneity on the effective growth kinetics of microorganisms in large scale modelling of porous media

Author: Ali Mahmoodi[1]

Co-author: Hamid M. Nick [2]

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Various microorganisms, such as Sulfate Reducing Bacteria (SRB), live in underground reservoirs. The growth rate of microorganisms in a reservoir is highly dependent on various parameters (e.g., the concentration of the nutrients and inhibitors, temperature, pH, and salinity). Especially in case of waterflooded hydrocarbon reservoirs, for large scale modelling of microbial processes, it is close to impossible to capture the exact distribution of these parameters without a certain level of simulation grid refinement, which increases computational costs, and without an accurate knowledge and definition of the distribution of static parameters in the model that control flow properties, such as heterogeneity in permeability distribution in various scales and the presence of fractures. Moreover, the distribution of the parameters affecting microbial growth in a reservoir is highly dependent on geochemical and thermal processes. For instance, the chemical interactions between reservoir fluids and rock (e.g., adsorption and desorption) under varying temperature can affect the concentration of nutrients and inhibitors for microbial processes as well as the measured produced water or gas compositions used for history matching. Geochemistry can also control the pH of the medium, which in turn affects the growth kinetics of microorganisms, the speciation of chemical species in the water phase, and the partitioning of chemical species among phases. The interconnected interactions among biological, hydrological, and geochemical processes as well as numerical challenges of nutrients and heat transport in large-scale models makes modelling and validating microbial growth in field scale particularly challenging.

This study demonstrates such challenges and presents a mathematical approach for upscaling microbial growth rates that corrects the effect of grid size on nutrient and temperature distribution in the reservoir and the corresponding effective growth rates. Moreover, the common way of representing fractures in field models using commercial reservoir simulators is re-evaluated, and it is shown how it can result in misleading reservoir models if the history matching is done using only production rates and pressure, neglecting the chemical composition of the produced water. Furthermore, the most important parameters in the model that highly affect the quality of the predictions are identified and proposed as research gaps for future experimental measurements.

The results show good predictions of upscaled (effective) microbial growth rates corrected for the effect of grid size on temperature distribution in course-grid simulation compared to refined simulation using non-upscaled growth rates. Moreover, it is demonstrated how the effective microbial growth behavior in presence of a fracture varies with the refinement level of the system and the method used to define the fracture in the model when the fluid production, pressure, and composition data match.

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Poster / 731

The emulsification phenomenon of heavy oil in porous media studied by nuclear magnetic resonance method.

Authors: Jiajing Chang[1]; Zhaojie Song[2]; Bingyu Ji[3]; Zengmin Lun[3]; Yongqang Tang[3]; Yibin Qi[3]; Zhaoyu Fan[2]; Kaixing Zhang[2]

[1] *China University of Petroleum, Beijing & Sinopec Petroleum Exploration and Production Research Institute, Beijing, China*

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Emulsification phenomenon is common in the displacement process of water flooding, surfactant flooding and multiple compound flooding in heavy oil reservoirs. The existence of emulsion can greatly improve the oil displacement efficiency, which has important practical significance for the development of heavy oil reservoirs. However, the description of emulsification phenomenon is basically based on the observation of produced fluid and the monitoring of pressure points along the way. The real emulsification situation in porous media cannot be observed. We have tested and analyzed the emulsification phenomenon of heavy oil in porous media by nuclear magnetic resonance experimental method.

In this study, D-T2 two-dimensional spectrum scanning was first performed on equal volume of free water, water-in-oil emulsion and oil-in-water emulsion. Secondly, the same volume of water-in-oil emulsion and oil-in-water emulsion were scanned by D-T2 two-dimensional spectrum at three different temperatures. Finally, the 60-mesh quartz sand was used as the porous medium, which was filled into the non-magnetic sand filling tube, and the equal volume of water-in-oil emulsion and oil-in-water emulsion were injected respectively. The D-T2 two-dimensional spectrum of the emulsion in the porous medium at different temperatures was tested.

The results showed that the water signal fell on the free water line in the D-T2 two-dimensional spectrum of free water. In the D-T2 two-dimensional spectrum of water-in-oil emulsion, water was limited by the dispersed phase droplets, and the water signal fell below the free water line. In the D-T2 two-dimensional spectrum of the oil-in-water emulsion, the degree of water diffusion was not limited, and the water signal deviated not far from the free water line. The higher the temperature, the formation of water-in-oil emulsion was more conducive, but it would reduce the stability of oil-in-water emulsion. The existence of porous media would make the stability of water-in-oil emulsion worse, and the higher the temperature, the stability of it was worse. However, the presence of porous media would lead to a decrease in the relaxation time of the aqueous phase in the oil-in-water emulsion, and the confined diffusion of the aqueous phase was not obvious under different temperature conditions.

This new experiment provides a new method and theory for studying the emulsification of heavy oil

in porous media. And its results can more accurately predict and guide the production of condensate gas reservoirs.

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MS07 / 734

Multiscale modeling of multiphase compressible non-isothermal fluid flow in deformable porous media

Author: Xiaojin Zheng[1]

Co-author: Ian Bourg [2]

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[2] *Department of Civil and Environmental Engineering, Princeton University, Princeton, NJ 08544, USA; High Meadows Environmental Institute, Princeton University, Princeton, NJ 08544, USA; High Meadows Environmental Institute, Princeton University, Princeton, NJ 08544, USA*

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Understanding the coupling between multiphase fluid flow in pores with distinct sizes and solid deformation induced by flow or external stresses is crucial for the development of many important geotechnics. Most well-established models for describing coupled fluid-solid mechanics are not capable of characterizing hybrid-scale systems containing both solid-free regions and porous media. The recent so-called Darcy-Brinkman-Biot (DBB) framework, which is based on the well-known Darcy-Brinkman equation and utilizes a unique set of volume-averaged partial differential equations, can capture capillary, viscous, inertial, interfacial, and gravitational forces at both the pore and Darcy scales. The solver tends asymptotically to the solution of the two-phase Navier-Stokes equations when used as a pore scale model and to the solution of the two-phase Darcy equations when used as a continuum scale model. Previous extensive tests have demonstrated the versatility of this solver to model multiscale multiphase flow in deformable porous systems, such as fluid-induced material deformation and failure.

In this work, we build upon these previous studies to extend the DBB framework to compressible non-isothermal fluid flow. Through careful addition of new energy conservation equations and pressure equations, we show that this new solver can predict heat transfer in compressible fluids and deformable solids. The model's numerical implementation, hybridBiotThermalInterFoam, is achieved in the Computational Fluid Dynamics (CFD) software OpenFOAM. This model is then rigorously validated via an example application in the engineered barrier system (EBS) in a nuclear waste repository. Results show that the new solver is capable of predicting fracture propagation and healing in bentonite buffers exposed to strong thermal fluxes and complex aqueous chemistry conditions.

The disjoining pressure and complex rheology of the clay matrix are explicitly represented as a function of porosity and salinity. This setting enables the application of thermo-poro-plastic relations to predict the potential for EBS fracturing. Finally, the predictions generated by this model are cross-validated against other existing THMC simulators and experimental measurements. The development in this work creates the first model representing multiphase compressible non-isothermal fluid flow in multiscale deformable porous media.

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Poster / 735

Exploring the Relation Between Soil Salinity on Soil Organic Carbon Dynamics in Global Terrestrial Ecosystems

Authors: Amirhossein Hassani[1]; Pete Smith[2]; Nima Shokri[3]

[1] *The Climate and Environmental Research Institute NILU*

[2] *University of Aberdeen*

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Soil Organic Carbon (SOC) is a fundamental component of terrestrial ecosystems, connected to climate regulation, nutrient cycling, and soil health. The influence of soil salinity - referring to the concentration of soluble salts in the soil solution - on SOC content is acknowledged (1,2), but there is limited understanding regarding the precise direction and extent of SOC's response to varying levels of soil salinity in real field conditions. This study explores the relationship between soil salinity and SOC content, necessary for understanding carbon sequestration processes, climate change mitigation, and terrestrial carbon stock stability. Using the SOC of 60,392 soil samples collected globally since 1950, we developed a statistical model (General Additive Model) and analyzed soil salinity's relation with SOC dynamics while controlling the role of other environmental parameters. According to the results of the statistical analysis, we estimate that an increase in soil salinity from 1 to 5 dS m-1 would be correlated with a decrease in SOC, equivalent to dropping from 0.92 g kg-1 above the mean predicted SOC (31.77 g kg-1) to 6.34 g kg-1 below the mean predicted SOC (-700%), while considering other influencing environmental factors such as precipitation and temperature. Our results show the minor contribution of salinity to SOC while other factors such as climate, vegetation, and land management practices exert more substantial effects on SOC content. Key covariates in relation with SOC include soil nitrogen, anthropogenic phosphorous input, and soil pH. Additionally, our study estimates the effects of one standard deviation increases in soil salinity of the analyzed soil samples on topsoil (0 –20 cm) SOC content, showing a 6.98% decrease in SOC. These findings highlight the importance of considering diverse factors in understanding SOC dynamics, providing insights into mitigating the impacts of soil salinity and climate change on terrestrial ecosystems.

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References:

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MS17 / **736**

Elastic properties evolution of carbonate rocks during reaction induced by carbon dioxide injection

Authors: Rui Li[None]; Yi Yang[1]; Yingfang Zhou[1]; Yuxuan Zhang[1]; Zaibin Lin[1]

[1] *University of Aberdeen*

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The sequestration of carbon dioxide in deep underground reservoirs is proposed as a strategy to alleviate atmospheric greenhouse gas emissions. Upon introduction into the host brine, carbon dioxide dissolves, creating an acidic solution. This acidity can subsequently engage with the host rock, prompting dissolution, particularly in carbonate formations. The mechanical change of host rock brought by this dissolution could be evaluated by the change of elastic properties(bulk and shear modulus). We performed pore scale simulations to examine the alterations in the micro-structure of rocks induced by the injection of CO_2-saturated brine, focusing on understanding the consequential evolution of the elastic properties of carbonate rocks. We modeled the evolution of the pore structure during dissolution by Volume of Solid method(VoS method), a finite volume method, and then calculated the changes in elastic properties by finite element method, combining with the effective medium theory. During our simulation, estaillades carbonate core is injected with CO_2-saturated brine at 50 ℃ and 10 MPa. After determining the accuracy of the simulation by comparing the reaction rate with that of the experiment under the same conditions, the changes in elastic properties was calculated. The efficiency of the VoS method lies in its computational simplicity, eliminating the need for remeshing or any specialized handling of topological changes.

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737

Modeling and effects of evaporation kinetics on mass transfer and salt precipitation during CO2 sequestration

Author: Boris Jammernegg[None]

Co-authors: Bernd Flemisch [1]; Denis Martynov ; Holger Ott [2]; Katharina Heck [3]

[1] *University of Stuttgart*

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Geological storage of CO2 is currently considered the most promising large-scale option to avoid emissions by industrial activities. Oil and gas reservoirs and the more abundant saline aquifers are regarded as suitable subsurface storage containers. The injection of dry or under-saturated supercritical CO2 into water-bearing formations leads to the formation of a so-called dry-out zone due to evaporation of the resident brine into the injected fluid and, hence, potential precipitation of formerly dissolved brine constituents. If minerals precipitate within the pore space of a rock formation, porosity and as a consequence permeability are adversely affected, which potentially impairs injectivity. Even though injectivity impairment poses operational and financial challenges, major questions remain unanswered; what is the size of the affected zone itself? What is the impact of capillarity on the fluid transport therein?

Current reservoir simulation tools lack in the description of mutual mass transfer of the involved fluid phases, which may lead to a significant misjudgment in terms of salt precipitation and the consequential clogging of the pore space. We developed a novel reservoir simulation module based on DuMuX capable of describing both evaporation and reaction kinetics.

In this presentation, the responsible evaporation of brine and fluid transport mechanisms are outlined and discussed, as well as the potential reduction of the formation permeability and with it the injectivity. Further, we will give insights into the implementation of the mass transfer between the fluid phases involved and the numerical model itself. A remaining important question is the zone of counter-current flow in the direction of the wellbore, which determines the amount of salt that potentially precipitates in the near-wellbore area and the accompanied porosity reduction.

We approach this question with numerical simulations to determine the size of the zone affected by the undersaturated CO2. The modified saturation profile in this zone allows for salt to be transported toward the injector. We investigate the major parameters governing this zone and the fluid transport therein. In parallel, we built up a meter-scale core flood experimental setup to extract fluid saturation profiles and solid saturation (precipitation) via CT imaging of core samples. Besides that, by monitoring the differential pressure, we can determine changes in permeability and, with it, changes in injectivity. In the next step, the gathered experimental data allows us to calibrate our numerical model and to upscale the results to the field scale. Anyhow, the experimental work is currently in progress. We will give insights in the future implementation.

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Poster / 738

Direct numerical simulation of CH4 - CO2 mixture flow in nanoporous media

Author: Chenyue Xie[1]

Co-authors: Jingwei Huang [1]; Xiaolong Yin [2]; Hui Zhao [3]

[1] *China University of Geosiences (Wuhan)*

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[3] *School of Petroleum Engineering.Yangtze University*

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CO2 injection into shale is believed beneficial for both enhanced gas recovery and CO2 storage. The confined space and strong solid-molecule interactions in nanoporous media lead to different occurrence states of CH4 and CO2, causing the flow of CH4 - CO2 mixture in shale to deviate from predictions of continuum models. In this study, we employed a modified pseudo-potential based lattice Boltzmann (LB) model to study gas mixtures in nanoporous media. The mixed equation of state is used to calculate interaction force between gas mixtures. The solid-molecule interaction force is determined by comparing density profiles from LB simulation and molecular dynamics. The proposed method can model the flow of CH4-CO2 mixture in complex topological nanopores with various surface properties. Our results demonstrate that the Langmuir model and BET theory cannot accurately describe the adsorption isotherms of CH4 and CO2 in nanoporous media. The transport capacity of CH4-CO2 mixture in nanoporous media is found affected by surface properties. In organic nanoporous media, CO2 molecules tend to accumulate near the pore surface, hindering their flow compared to CH4 molecules. In contrast, inorganic nanoporous media facilitate the flow of both CH4 and CO2 molecules. We propose a modified apparent permeability model to describe the flow capacity of a CH4-CO2 mixture in nanoporous media.

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MS09 / **739**

Effect of roughness in the fluid flow in porous media: based on random fields theory and 3D printing technology

Author: Yunlong Wu[None]

Co-authors: Jean-Baptiste Colliat ; Jean-Philippe Carlier [1]; Nicolas Bur

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The morphology of pores is an important factor influencing the permeability of porous materials[1,2,3]. In recent decades, the influence of the morphology of pores on fluid flow in geomaterials has attracted extensive attention in the engineering fields of petrochemistry, hydrogeology, civil and geotechnical structures, with applications in radioactive hazardous waste storage[4], oil and gas storage[5,6,7], carbon dioxide sequestration[8], and geothermal energy extraction[9].

To model porous media whose morphology is precisely controlled, excursion sets of random fields have been used recently[10]. The models generated by this method have the advantages of isotropy, ergodicity, generalizability, stability, and controllability. In previous studies, researchers have focused on generating correlated random fields using the Gaussian covariance function. However, the actual pores are not smooth.

To explore the effect of roughness on fluid flow within porous media, in our research, the Matérn covariance function has been chosen to describe the random field. The Matérn covariance function allows controlling the level of smoothness, which can be adjusted by a parameter ν greater than 0[11]. Using this function, a three-dimensional continuous field can be generated. Afterwards, to transform this continuous field into a binary field with only matrix and pores, the excursion set method is used. This method transforms the continuous field into a binary field with varying volume fractions by selecting different threshold values. Therefore, by controlling the threshold value, the porosity of the generated porous medium can be precisely controlled.

By the above methods, models of porous media whose roughness is precisely controlled are generated. In order to relate the parameter ν to common roughness parameters, we analyze the fractal dimension and the specific surface area of the generated field and compare the relationship between them. Afterwards, to analyze the effect of roughness on fluid flow, experimental and numerical investigations have been performed.

In terms of testing, a number of samples with different roughnesses were generated using SLA 3D printing, which printing accuracy can reach 50 microns. To verify the accuracy and the quality of the 3D printed samples, the samples were characterized by micro-CT technique. By comparing the scanned images with the numerical model, the parameters such as porosity, pore connectivity, fractal dimension, tortuosity, and specific surface area were analyzed. Subsequently, the permeability of each sample was measured through Darcy tests, and the correlation between permeability and roughness was analyzed.

In order to compare with the experimental data, numerical simulations were performed using the lattice Boltzmann method[12], using the Palabos library[13]. This method has advantages in dealing with complex boundaries and parallel operations, which is very suitable for porous media models. Considering factors such as stability and applicability, the D3Q19 lattice model was selected. The numerical model of all the samples used in the test was considered, the fluid flow in the porous medium was simulated under the same conditions in the test, and the flow rate and permeability were calculated.

Finally, the results of the test and simulation were compared and analyzed, and a law describing the evolution of permeability with roughness was proposed.

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MS13 / 741

Multicomponent alkanes transport through nanoporous shale matrix

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Shale is attracting more and more attention owing to the huge hydrocarbon resources. However, the large number of nanopores and the multiscale pore structure pose great challenges in accurately characterizing the transport behavior of crude oil within the shale matrix. Although most studies suggested that the classical Darcy's law breakdown in the shale matrix, there is a great controversy on the oil transport mechanism: slip flow or the existence of stick layers, which impedes the efficient exploitation of shale oil. To address this issue, we study the transport of multicomponent alkanes through a nanoporous shale matrix by integrating molecular dynamics and digital rock. We consider the multi-component characteristics of shale oil and the typical mineral composition of shale reservoirs. Firstly, we use molecular dynamics to accurately capture the pressure-driven flow behavior of multi-component alkanes within kerogen cylindrical pores and calcite nanoslits, from which a mathematical model is developed to characterize the transport behavior. Then, based on Focused Ion Beam Scanning Electron Microscopy (FIB-SEM) images, we build an ultrahigh-resolution digital rock model using deep learning. A pore network model is extracted from this digital rock and used for the flow simulation of crude oil through the shale matrix. For the molecular studies within a single nanopore, we reach the following conclusions: sticky layers, whose velocity approximates zero, exist during oil flow through kerogen and calcite nanopores. Oil adheres onto the shale surfaces for the smaller driving force, resulting in a sticky layer that impedes flow. As the driving force increases, certain alkane molecules surpass the affinities from the rock surface and facilitate the flow, leading to a thinner sticky layer. The heavier components in shale oil show stronger interactions with rock surfaces, making them highly susceptible to adsorption and the sticky layer. Moreover, the thickness of the sticky layer in kerogen pores is greater than that of calcite nanopores, which can be attributed to the atomic roughness and fluid-solid interactions. Based on these findings, we have developed a mathematical model that describes the variations in the sticky layer thickness within different pores with respect to parameters such as driving force, alkane components, and pore size. Even with the assistance of FIB-SEM, the observation of shale nanopores smaller than 10 nm is challenging, which leads to the unreliable assessment of shale pore network connectivity. We develop a stepwise 3D super-resolution reconstruction method for shale digital rocks based on deep learning, which significantly improves the accuracy of digital rock core and enables successful observations of pores smaller than 10 nm. We then use the pore network model to simulate shale oil flow at the pore scale. Our findings showed that the transport of oil through the shale matrix is nonlinear and has a threshold pressure gradient due to nanoscale sticky layers. When the displacement pressure gradient exceeds the threshold pressure gradient, oil starts to flow and lighter components dominate shale oil transport. This study sheds light on the accurate modeling of shale oil production and more generally, for mass transport in nanoporous materials.

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Poster / 742

Simulation of multiphase porous media flow in acid stimulation formations with an adaptive mesh refinement strategy

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In our previous work, we investigated the fingering behavior in acid stimulation formations and found that the dissolution patterns in acid stimulation region have an influence on the injection performance. A detailed characterization of the highly heterogeneous wormholes could introduce a large number of gridblocks and subsequently increase the computational burden drastically. In this work, an adaptive mesh refinement strategy is proposed for a computationally efficient simulation of multiphase porous media flow in acid stimulation formations. As a preprocessing step, we construct multiple tiers of grids containing the heterogeneous features in the vicinity of the wellbore and ascertain their topology. The saturation is taken as a criteria during simulation to switch the grids locally. When the saturation of the injected phase is lower than a threshold value, a fine grid is used to capture the fingering behavior. When the value is surpassed, a coarse grid is used instead. With respect to the switch, the upscaling is achieved using a volume weighted approach, while the downscaling is achieved using a basis function interpolation method. A number of scenarios are used to evaluate the technique, and the results demonstrate its feasibility, strong computational performance, and accuracy.

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MS18 / 743

Numerical modeling of the PFAS Fate in a Former Firefighting Training Site in Korsør, Denmark

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The extensive use of products containing high concentrations of Per- and Polyfluoroalkyl Substances (PFAS) has led to the spreading of such “forever chemicals”in soil and groundwater In certain locations, like Korsør in Denmark, a former firefighting training site, PFAS have been detected in the vadose zone in measurable amounts 1. Studies in such areas are crucial for understanding the PFAS

behavior in subsurface soil layers.
This numerical model focuses on the transport behavior of four PFAS (per-fluoro butanoic acid-PFBA, per-fluoro octanoic acid-PFOA, per-fluoro decanoic acid-PFDA, and per-fluoro octane sulfonic acid-PFOS) in the vadose zone, with emphasis placed also on potential PFAS leaching into groundwater. For this purpose, a 3D domain has been constructed, with dimensions 8 m in depth and area 100m2 consisting of multiple soil layers with various initial water saturation levels (Figure 1). The great variety of soil types necessitates enhanced model accuracy 2, achieved through a Python code that analyzes the geological layers of the site. This code interprets different colors in the geological model (each color representing a distinct soil layer) as layers of varying permeability and effective diffusivity, by utilizing background knowledge from literature [3].

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In this study, the Richards equation is employed to model fluid transport within unsaturated porous media in the COMSOL platform by utilizing the Multiphysics module [4]. This equation is integrated with the van Genuchten approximation [5] for defining relative permeabilities in relation to effective saturation.
In addition to the well-known transport mechanisms, such as convection, diffusion, and dispersion, PFAS adsorption plays a significant role in the retention process [6]. The present approach considers that PFAS adsorption occurs on both the solid grain-water interfaces and the air-water interfaces. The PFAS sorption coefficients on air/water interfaces were estimated by fitting curves of the water/air surface tension as function of PFAS concentration with the Langmuir-Szyszkowski equation or were taken from literature [7]. The kinetics of PFAS sorption on solid/water interfaces was estimated with inverse modeling of the relevant breakthrough curves of soil column experiments or were taken from literature [8].
The spatial-and-temporal distribution of the concentration of four PFAS compounds (PFBA, PFOA, PFOS, and PFDA) is detected as they percolate through the vadose zone until reaching the aquifer by accounting for the unique properties of each PFAS [8]. Multiple scenarios are tested, starting with the initial state of soil (whether saturated or unsaturated) and extending to various soil types, different initial PFAS concentrations, and varying precipitation rates. Precipitation plays a crucial role as it stimulates the convection mechanism. Additionally, the retention factor is estimated to be significant, particularly as the initial PFAS concentration increases. The different scenarios of PFAS motion in subsurface have generated insightful results, regarding strategies for soil treatment.
Acknowledgments
This work was performed under Grant Agreement 101037509 —SCENARIOS —H2020-LC-GD-2020 / H2020-LC-GD-2020-3 (project title: “Strategies for health protection, pollution Control and Elimination of Next generAtion RefractIve Organic chemicals from the Soil, vadose zone and water”-acronym “SCENARIOS”) supported by the European Commission.

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MS01 / **744**

Pore-Scale Dynamics in Carbonate Reservoirs: Understanding Heterogeneity's Influence on CO2 Storage in Indiana Limestone

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Co-authors: Catherine Spurin [2]; Martin Blunt [1]; Ronny Pini [1]; Sam Krevor ; Sojwal Manoorkar [3]; Steffen Berg [4]

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Subsurface carbon dioxide (CO2) storage is one of the most critical strategies in combatting climate change. One of the principal challenges encountered by the Carbon Capture and Storage (CCS) industry is the accurate understanding, representation, and upscaling of fluid flow dynamics within targeted reservoir formations. This problem is rather complex in carbonate formations due to their varying spatial heterogeneities and complex pore structures. In our experiment, we assess the impact of microporosity, heterogeneity and connectivity on saturation changes, and trapping in Indiana limestone samples.

We image Indiana limestone core samples using a high-resolution μCT scanner, with a resolution of 4.9 μm. Through two cycles of drainage and imbibition, we flooded the core with two different flow rates, to understand the influence of heterogeneity on the mobility of both wetting and non-wetting phases within the porous media. During the two cycles, the pore-scale capillary number was kept well within the capillary flow regime (10-7 - 10^-8). Our study highlights noticeable differences in saturation, non-wetting connective path, and dynamics of pore-filling between the two flooding cycles. Additionally, we show the redistribution of the non-wetting phase across the pore space when increasing the non-wetting phase flow rate. Furthermore, we investigate intermittent flow observed during imaging manifesting as artefacts within the reconstructed 3-D volume. This exploration aims to elucidate the origins and implications of intermittency, providing valuable insights into its impact on imaging quality and interpretation of pore-scale fluid dynamics.

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Poster / 745

Mass transfer across fracture-matrix interface in a flowing fracture

Author: Mohsen Farhadzadeh[1]

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Mass transfer across fracture-matrix interface in a flowing fracture
Mohsen Farhadzadeh, Hamid M. Nick

A direct numerical simulation of the Navier–Stokes equations is utilized to solve two-phase flow in simple fractured porous media 1. We focus on understanding the impact of fracture flow on the mass transfer between the fracture and porous matrix utilizing a two-dimensional geometry consisting of a single fracture with a limited number of pores.
We illustrate different imbibition regimes during water injection through the fracture into the porous domain saturated with oil. The impacts of contact angle, viscosity ratio, and interfacial tension for variable injection rate on the mass transfer across the fracture-matrix interface are analyzed. The simulation results suggest the fracture flow rate controls the rate of fluid phase transfer between the fracture and matrix domains.

Reference:
Farhadzadeh, M., & Nick, H. M. (2023). The critical role of fracture flow on two-phase matrix–fracture transfer mechanisms. Advances in Water Resources

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746

A Novel GPU-accelerated NMR T2 Simulator Resolving Surface Roughness Effect

Author: Yiteng Li[1]

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1. OBJECTIVE/SCOPE
   Commercial digital rock physics software utilizes the random walk technique to simulate NMR T2 relaxation in digital rocks. However, the effect of surface roughness, which is manifested as irregular solid-pore interfaces at the resolution of micro-CT imaging, is often overlooked; as a result, the data interpreter may incorrectly characterize pore structures and misinterpret petrophysical properties. This work proposes an innovative GPU-accelerated simulator that explicitly resolves the surface roughness effect on NMR T2 relaxation.
2. METHODS, PROCEDURES, PROCESS
   This work aims to develop a GPU-accelerated NMR T2 simulator that effectively regulates the nuclear magnetization decay during random walk simulations. To determine the amount of corrections to decelerate the nuclear magnetization decay, the pore space of the digital rock is decomposed into a plurality of disconnected pore bodies using the SNOW algorithm. The relaxation correction factor is then defined to properly reduce the magnetization decay rate and is assigned back to solid voxels along the solid-pore interfaces. When a walker collides with a solid voxel, it accesses the local correction factor that affects the NMR magnetization decay locally. The heterogeneous roughness correction factors are then upscaled into a few representative values for practical applications.
3. RESULTS, OBSERVATIONS, CONCLUSIONS
   The accuracy and efficiency of the proposed NMR T2 simulator are first verified with commercial software. Without accounting for the surface roughness effect, our simulation results agree well with the results of commercial software. From the perspective of computational efficiency, the proposed simulator achieves two orders of magnitude speedup, which could be even more efficient for high-fidelity simulations in high-resolution digital rocks. The roughness correction factor effectively controls the accelerated surface relaxation, generating more accurate T2 responses for pore structure characterization. This demonstrates the importance of modeling the surface roughness effect on NMR T2 relaxation. With a proper upscaling scheme, we can obtain almost the same T2 relaxation times using a few representative correction factors rather than a fully detailed model. This signifies the importance of upscaling roughness correction factors for practical applications.
4. NOVEL/ADDITIVE INFORMATION
   We developed an innovative GPU-accelerated NMR T2 relaxation simulator, the first one in the petroleum industry that explicitly resolves the surface roughness effect. The proposed simulator provides an integrated platform for the accurate and effective characterization of pore structures from digital rock models.

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MS16 / 748

Evaporation and absorption of surfactant-laden droplets on unsaturated porous media

Authors: Xiaoxing Li[1]; Hans Kuerten[1]

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Understanding the evaporation and absorption of surfactant-laden droplets on porous media is challenging and important for many industrial applications, for example, inkjet printing. The evaporation of droplets containing dispersed solid particles on a solid surface has aroused much interest and has extensively been studied. The non-uniform evaporation pattern, resulting after evaporation, is well known as the coffee ring effect. Deegan et al. 1 found that this pattern is caused by the outward flow within the droplet during evaporation. To obtain a uniform deposition pattern, surfactants are added which suppress this outward flow, which is especially significant in inkjet printing applications to enhance the print quality.

The evaporation of surfactant-laden droplets on a fibrous thin paper sheet is a more complex process, involving spontaneous droplet evaporation, water imbibition into pores causing an unsaturated porous medium, and surfactant transport in both the droplet and the porous medium, as illustrated in Figure 1. We use both theoretical and numerical methods to explore this process. The mathematical model for flow in droplets is based on lubrication theory. For the calculation of the vapor concentration, which determines the evaporation flux, an analytical method is used. For the droplet absorption process, the Richards equation is used, where it should be noted that we do not describe the flow on the scale of the pores, but rather use properties averaged over a number of pores. For the surfactant transport process, a mass conservative convection-diffusion model is employed. A three-stage diagonally implicit Runge-Kutta scheme and a finite volume method are used to simulate the process numerically. We will specifically study how the results are affected by the assumption of unsaturated flow in the pores. We will validate the unsaturated flow model and simulation method by comparison with numerical solutions for transient flow in a thin porous medium obtained by Zhuang et al. 2

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1 Deegan, R. D., Bakajin, O., Dupont, T. F., Huber, G., Nagel, S. R., & Witten, T. A. (1997). Capillary flow as the cause of ring stains from dried liquid drops. Nature, 389(6653), 827-829. 2 Zhuang, L., Hassanizadeh, S. M., Bhatt, D., & van Duijn, C. J. (2021). Spontaneous Imbibition and Drainage of Water in a Thin Porous Layer: Experiments and Modeling. Transport in Porous Media, 139(2), 381-396.

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749

Streaming potential measurements in glass bead packs - Benchmarking zeta potential calculations

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Zeta potential is a well known parameter for the description of the surface charge. It is widely used for particle interaction description, dispersion stability and fluid-solid interaction.

There are different electrokinetic methods available to measure zeta potential. To obtain zeta potential of a consolidated porous medium, the streaming potential method is a logical choice. Although commonly used, no commercial set-ups are readily available for permeation mode of measurements where fluid flows within the sample. Anton Paar's SurPASS 3 TM as several modules available, equipped for powder and membrane measurements but measurements on consolidate samples are done in tangential mode, where fluid passes along the sample surface.

Most laboratories build therefore in-house set-ups \cite{1st,2nd,3rd,5th,6th}, where additionally to the standard core flooding set-ups, non-polarizing Ag/AgCl electrodes and a voltmeter are incorporated to measure voltage difference that arises over the core during fluid flow. The set-up needs to be insulating (no metal parts) and flow direction reversal is advised in order to achieve stable voltage measurements. The so-called streaming potential develops due to the shear of movable charge in the electric double layer and in combination with measured pressure drop gives the streaming coefficient used in the classic Helmholtz-Smoluchowski equation \cite{7th} to calculate the zeta potential. The formula is applicable to plate or capillary tube geometries, but attempts are made to extend this theory to porous media \cite{8th,9th,10th}.

In this work we present our study to benchmark our homemade set-up. Literature data shows non-unique data and a large scattering of data, within the range of solid composition, and measurement conditions of temperature, pH and conductivity. We compared results with other (commercial) set-ups using sodium chloride salt concentration dependence and bead size (150-500µm) using bead packs of soda-lime glass beads. Repeatability of data in one set was given. Comparability of values between set-ups was not given. Assuming glass beads are inert, no pH control was included. The glass beads however changed pH in each system differently dependent on the volume ratio liquid/beads, from 5,6 to maximum pH 10. Accurate reporting of all parameters is needed for comparison including pH, resistivity, conductivity and reporting of the solid composition. A downward zeta potential trend was found with decreasing bead size, see Figure ZP NaCl.png, which is not expected based on the theory including surface charge \cite{10th}. Based on glass plate measurements in a SurPASS 3 TM where the assumptions of Helmholtz-Smoluchowski equation are met, a correction is needed to reduce the zeta potential for smaller bead sizes. The work indicates that a comparison of zeta potential measurements of different sources using bead packs is not straight forward and the classic Helmholtz-Smoluchowski equation might need further adaptions.

figure: ZP NaCl.png
caption: The dependency of the calculated zeta potential from streaming potential measurements in glass bead packs on bead size and NaCl concentration, compared to glass plates. A clear downward trend with decreasing glass bead diameter is observed.

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MS06-A / 750

Mechanism of oil absorption in surface engineered sponges for wastewater treatment

Author: Gijs Wensink[1]

Co-authors: Pavani Cherukupally [2]; Laurenz Schröer [3]; Kobus van Kempen [1]; Job ten Hacken [1]; Veerle Cnudde [3]; Maja Rücker [1]

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Using porous materials for absorption of fluids has been practiced for thousands of years, for e.g. water storage and release and for filtration purposes. The chemical nature of the porous material and the flow dynamics determine how absorption takes place and which fluids are preferentially absorbed. In this way, materials can be designed for various fluid separation applications. In our work, we study the effects of the pore geometry on absorption of oil into surface engineered sponges. The sponges consist of a polyurethane based fiber network and contain a porosity of ~98%. The fibers are made hydrophobic by chemical functionalization for usage in wastewater filtration and oil spillage clean-up 1. They contain both pores in between fibers (inter-fiber pores) as well as within the fibers themselves (intra-fiber pores). We study the mechanism of the absorption process by

tracking dodecane (a hydrocarbon) invasion in 3D over time using dynamic micro-CT experiments. The experiments were performed within the EXCITE network using the EMCT scanner at University of Gent Center for X-ray tomography (UGCT).

In the visual experiments, we observe an initial precursor invasion of dodecane in pores in between fibers within a few hours, without invasion of the interior of the fibers. Likely, this precursor front is driven by a density difference between water and oil, since the front moves under positive curvature (i.e. against capillarity). This indicates an initially weakly water-wet nature of the fiber surface. Quantitative volumetric measurement data, through which we fit a two-term kinetic model, show a second main front of dodecane moving into the samples on a time scale of several days. The slower main front invasion is coupled to a change in the observed fiber wettability at the pore scale from water-wet to oil-wet over time.

In order to elucidate the absorption mechanism, we conduct separate experiments using dodecane emulsified in water. We observe a gradual uniform absorption of dodecane in intra-fiber pores, on which droplets of dodecane nucleate. These droplets grow over time, partially filling the inter-fiber pores. This effect shows us that the exterior of the fibers indeed likely change to an oil-wet state due to the invasion of oil into the fibers.

This research shows not only the significance of precursor fronts in fluid absorption processes in porous media, but also that they can be caused by gravitational effects instead of capillarity 2. The study results can be extended to porous media applications where a range of pore sizes can be expected, such as wastewater filtration, CO2 and hydrogen storage in porous reservoir rocks and paper wetting in inkjet printing.

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1 Cherukupally, P., Sun, W., Wong, A. P. Y., Williams, D. R., Ozin, G. A., Bilton, A. M., & Park, C. B. (2019). Surface-engineered sponges for recovery of crude oil microdroplets from wastewater. Nature Sustainability, 3(2), 136–143. https://doi.org/10.1038/s41893-019-0446-4; 2 Constantinides, G. N., & Payatakes, A. C. (2000). Effects of Precursor Wetting Films in Immiscible Displacement Through Porous Media. Transport in Porous Media 2000 38:3, 38(3), 291–317. https://doi.org/10.1023/A:1006557114996

Conference Proceedings:

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MS22 / 751

Characterization and numerical investigation of 3D-printed porous organic cages for gas adsorption

Author: Bin Ling[1]

Co-authors: Rishav Agrawal ; Robert J. Poole [1]; Donglin He [2]; Andrew I. Cooper [1]; Ming Liu [3]; Esther García-Tuñón [1]

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Porous organic cages (POCs) are a class of emerging microporous materials with high porosity and selectivity for gas adsorption and separation.1 As a representative of first-generation POCs, CC3 has huge potential for separating noble gases and volatile organic compounds (VOCs).2 Traditional manufacturing techniques exhibit some limitations in immobilizing the porous materials into structural adsorbents, such as poor transfer efficiency, insufficient loading of active material, limited structural forms, etc.[3] Three-dimensional (3D) printing demonstrates significant advantages in building complex structures with controlled features, to fully exploit their potential.[4] In this study, we demonstrate a versatile approach to 3D print porous materials, successfully shaping CC3 into hierarchically porous architectures by direct ink writing (DIW)[5]. Through the rational design of formulations, we obtained inks that combine both printability and functionality and printed a series of filter prototypes. The optimization of flow physics by tailoring the geometric parameters can effectively improve the contact, diffusion, mass transfer, and energy loss.[6] This is achieved by utilizing computational fluid dynamics (CFD) to numerically investigate the flow behavior and interactions through the structures for gas adsorption applications.[7]

The bentonite-based hybrid additive was used in the formulation as its unique layer structure constructs an interlinked network.[8] This brings the inks with good plasticity beneficial for printability and also retains active sites for CC3. The linear and nonlinear viscoelastic behavior of the inks with different CC3 loading (from 0wt% to 70wt%) were characterized by the oscillatory shear rheology to quantitatively study their printability. These inks were constructed into multiscale porous structures using DIW, and it was found that the crystal structure (Fig. 1a) and the adsorption capacity (Fig. 1b) of CC3 can be well preserved. The specific surface area is positively correlated with the loading amount of CC3, which can reach 249.35 m^2/g for 70wt% CC3 (Fig. 1b). However, the increase in CC3 content leads to a reduction in mechanical performance due to less shrinkage effect dominated by bentonite.[9]

Based on the printed structures (Fig. 1c and d), porous 2D repeating unit cells achieved with periodic boundary conditions with varying offset filament distance, pore size, and porosity were designed and simulated under different flow conditions using a commercial CFD package (Ansys Fluent). The extended Darcy-Brinkman-Forchheimer model was used to model the flow in the filament's porous zone.[10] The numerical results reveal that as the Reynolds number (Re) increases, a recirculation region develops and gradually expands within the gas flow path. Increasing offset distance brings more curved streamlines (Fig. 1e) and leads to a rise of pressure drop and overall flow resistance. The effect of filament's porosity and pore size on the pressure drop is investigated. This work provides a pathway for designing and fabricating high-performance adsorption systems, and can also be widely used for other functional materials for sustainable environment and energy applications.

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MS12 / **752**

Micromechanical Coupling of Irregular Particles and Fluid

Author: Pejman Tahmasebi[1]

[1] *Colorado School of Mines*

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Exploring the complex interplay between granular materials and accompanying fluids is an intricate problem, as their morphological properties add layers of complexity to the interplay of inertial, viscous, frictional, and elastic forces, which can make modeling such systems difficult. Here, we introduce a novel coupled framework designed to study the impact of particle morphology on granular particle dynamics. Our micro-mechanical model sheds light on the mechanical behavior, revealing significant influences from particle morphology. Interestingly, the presence of fluid mitigates movement differences induced by particle shape. Demonstrating these insights through a collapse process, we observe that the fluid's viscous and lubrication effects distinctly hinder and enhance dislocation, respectively. Notably, the dominance of fluid lubrication intensifies with increasing irregularity in particle shapes.

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MS03 / **753**

Experimental study on the effect of supercritical CO2 and acid alternative injection mode on the acid-etching behavior and conductivity of fracture in carbonate rocks

Authors: Bo Gou[1]; Ke Xu[1]; Jianchun Guo[1]; Xiao Li[1]; Mingwei Lei[1]; Junshuo Zhang[1]

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In order to enhance acid penetration depth and fracture conductivity, acid fracturing techniques involving the alternating injection of non-reactive fluids (fracturing fluids) or weakly reactive fluids (self-generated acid) with acid are considered a pivotal enhanced oil recovery rate in carbonate reservoirs. In recent years, the CO2-enhanced acid fracturing technique has gained prominence in the Middle East. This method adopts a mixed injection mode of CO2 and acid liquid in the wellbore, featuring the advantageous effects of retarding acid-rock reaction rates, improving fracture conductivity, and conserving water. However, its application in deep wells is limited by the high friction associated with the mixture of CO2 and acid. Supercritical CO2 and acid alternating injection, conducted under the conditions of conventional acid fracturing with established dominant fracture channels, involves supercritical CO2 injection to reduce the flow resistance of CO2 into the reservoir, showcasing potential for application in deep wells. Nevertheless, the impact of supercritical CO2 and acid alternating injection on hydraulic fractures and conductivity has not been reported.

This paper utilizes a self-developed supercritical CO2 acid etched fracture conductivity simulation device and employs downhole cores to conduct experiments on hydraulic fracture acid etching and conductivity under two scenarios: alternating injection of weakly reactive fluid (self-generated acid) with gelled acid and alternating injection of supercritical CO2 with gelled acid.

Research results indicate that supercritical CO2 and gelled acid alternating etching exhibits more pronounced elevation variations on the fracture surface, demonstrating a stronger and more dispersed non-uniform etching compared to the self-generated acid/gelled acid alternating injection mode. In terms of fracture conductivity, CO2/gelled acid alternating injection exhibits higher initial fracture conductivity, and under medium to high closure pressures (≤52MPa), self-generated acid/gelled acid alternating injection demonstrates higher conductivity. However, at high closure pressures (>52MPa), the supercritical CO2/gelled acid alternating injection mode can create higher fracture conductivity.

This study experimentally explores the impact of supercritical CO2 and acid alternating injection on fracture conductivity, demonstrating that for deep carbonate reservoirs with high closure stress, adopting this mode has the effect of reducing the usage of non-reactive or weakly reactive fluids and enhancing fracture conductivity under high closure pressure.

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754

Microscale simulation of reactive flow in particulate filter based on tomography images

Authors: Liu Tao[1]; Pavel Toktaliev[2]; Oleg Iliev[None]; Martin Votsmeier[1]

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Reactive flows in porous media constitute integral components of numerous industrial processes, exemplified by their role in particulate filter systems within the automotive sector. A crucial aspect in comprehending transport phenomena at the microscale involves the numerical simulation of species transport, particularly in the context of CT scan geometry. However, the inherent limitation of CT scans, characterized by insufficient resolution, may obscure or leave unresolved various features of microscale flow and transport. In this study, we prepared and subjected an SCR Diesel Particulate Filter (SDPF) sample to scanning, achieving a voxel resolution of approximately 360 nm. This resolution enabled the discernment of voids within the washcoat. Subsequently, a down-sampling method was employed to reduce the computational domain size while preserving the main features of the model. Validation was conducted on both the original and down-sampled geometries, resulting in a satisfactory agreement. With the validated models, a series of parametric studies were conducted to explore the impact on washcoat performance. The findings indicate that a decrease in the washcoat diffusion coefficient does not significantly influence overall conversion but does affect washcoat efficiency. Inlet velocity affects species conversion, albeit with minimal impact on washcoat efficiency. The micro-morphology and structure of the washcoat emerge as pivotal factors influencing both conversion and washcoat efficiency. The porous morphology facilitates gas entry into the washcoat, thereby mitigating mass transfer limitations. These results contribute to a deeper understanding of transport processes in particulate filters at the microscale, offering valuable insights for the design and optimization of particulate filters.

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MS09 / **755**

Direct pore-scale modeling of foam flow through 3D rough fractures

Author: Xuesong Ma[None]

Co-authors: Bernard Chang ; Masa Prodanovic

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Foams are dispersions of gas bubbles within a liquid. They can be generated in porous and fractured media during co-injection of two fluids in the presence of surfactants that stabilize foam bubbles. Since foam viscosity is much higher than the constituent gas and liquid phases, they are used for diverting fluid to less permeable subsurface formations in applications such as enhanced oil recovery or carbon dioxide storage. Pore geometry, thermodynamic conditions, molecular structure and behavior of stabilizing agents such as surfactants or nanoparticles near fluid/fluid or fluid/solid interfaces are some important factors affecting stability and regeneration of foam in porous media.

We present the first 2D and 3D results from a direct pore-scale modeling of foam in porous media. We use free-surface lattice Boltzmann method adapted for simulation in an imaged realistic fracture geometry. All geometries are available from Digital Rocks Portal, https://www.digitalrocksportal.org/. The model couples Navier-Stokes equation for fluid flow between bubbles and diffusion of dissolved gas within liquid into bubbles, and is adapted from LBfoam (https://github.com/mehdiataei/LBfoam) open solver that originally does not account for porous medium. To our knowledge, this is the first 3D model with the foam flow driven by pressure gradient in a fractured porous medium, gas diffusion through liquid phase and the interface changes as a result of both aforementioned mechanisms at pore scale. The bubble morphological variations we observe are caused by bubble coalescence, splitting and merging and we quantify them using morphological parameters (Minkowski functionals) in different liquid viscosity, pressure gradient, surface tension and temperature conditions.

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Poster / **757**

Coupling Deep Learning with Progressive Growing Generative Adversarial Networks and Data Assimilation for Inverse Modeling in Complex Aquifers

Author: Liangping Li[1]

Co-author: Michael Tetteh

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The presence of hard data in geostatistical modeling and optimization problems is important in performing efficient parameter estimation. The hard data at specified points in the model domain serve as a guide in optimizing the unknown parameters to follow the patterns of the hard data. Recently, a novel approach to solving hydrogeologic/reservoir modeling problems has emerged by using deep generative models, specifically generative adversarial networks (GANs), to generate realistic and diverse images of channelized aquifers. This subsequently can be coupled with other geostatistical methods to solve parameter estimation problems. This study focused on using an improved GAN, called a progressive growing generative adversarial network (PGGAN), conditioned with hard data to perform parameter estimation of complex facies models by coupling an ensemble smoother with multiple data assimilation (ES-MDA). First, the PGGAN was trained to an image with 128×128 resolution in this work. The trained PGGAN was used to generate hydraulic conductivity fields when fed an ensemble of latent variables and hard data. The ES-MDA then was used to update the latent variable with the help of hydraulic head data obtained from the groundwater model. The approach was evaluated by using a synthetic example of the groundwater flow model a reference facies model randomly cut from the training image. Results show that this approach was able to perform efficient estimation of an unknown facies model domain. The results also show that coupling of PGGAN and

ES-MDA conditioned to both hard data and hydraulic head data was able to reconstruct the complex channel structures of the randomly cut facies model from the training image and reduce the uncertainty of the predictions.

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Poster / 758

Multi-scale flow, permeability, and heat transport in building materials

Authors: Hannah Menke[1]; Julien Maes[1]; Kamaljit Singh[1]; Katherine Hood[2]

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Permeability and heat transport through building materials ultimately dictates their insulatory performance over a buildings service lifetime. However, characterisation of building materials is challenging because porous building materials are heterogeneous and their macroscopic physical properties (e.g. permeability, thermal, and mechanical) depend on their micro scale characteristics, i.e. the local distribution and features of the solid components and the connectivity of the spaces between them. Large-scale testing can measure these macro-scale properties, but often does not give insight into the underlying micro structural properties that ultimately leads to optimisation. Thus, a knowledge of the 3D structure is therefore required to assist in the development and implementation process for new materials. Experiments combining X-ray microtomography with numerical modelling are an accepted method of studying pore scale processes and have been used extensively in the oil and gas industry to study highly complex reservoir rocks. However, despite the obvious similarities in structure and application, these techniques have not yet been widely adopted by the building and construction industry.

We have investigated the pore structure of several building materials, both conventional and historic using X-ray tomography and direct numerical simulation. Five samples were imaged at between a 4- and 15-micron resolution inside a micro-CT scanner. The porosity and connectivity were extracted with the grain, throat, and pore size distributions using image analysis. The permeability, velocity, and thermal conductivity were then investigated using GeoChemFoam, our highly versatile and open- source numerical solver. We found that each material had a unique, heterogeneous, and sometimes multi-scale structure that had a large impact on the permeability and thermal conductivity [Figure 1]. Furthermore, we found that the method of including sub resolution porosity directly affected these bulk property calculations for both parameters, especially in the materials with high structural heterogeneity. This is the first multi-scale study of structure, flow and heat transport on

building materials and this workflow could easily be adapted to understand and improve designs in other industries that use porous materials such as fuel cells and batteries technology, lightweight materials and insulation, and semiconductors.

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Figure 1: The local heat flux (J) through Bentheimer building stone (left) and a historic brick (right).

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MS11 / 759

Validation of methodology for MMP measurements on microfluidic slim-tube analogue

Authors: Evgeny Shilov[1]; Dmitrii Pereponov[1]

Co-authors: Michael Tarkhov [2]; Vitaly Kazaku [3]; Ivan Filippov [2]; Alexander Rykov [2]; Andrey Betekhtin [4]; Ivan Promzelev [4]; Vladislav Krutko [4]; Alexey Cheremisin [1]

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The industry-accepted standard to define the necessary conditions for miscible oil displacement by gas is the laboratory slim-tube test, which lasts over one month and requires much fluid to be tested. This research aims to validate the results of experiments on microfluidic slim-tube analogues for the determination of minimum miscibility pressure (MMP) and propose a novel methodology to overcome the drawbacks of the traditional method. The porous structure of the microfluidic chip used in this study is represented by a channel filled with cylinders randomly distributed along it. The silicon-glass microfluidic chip and the special microfluidic platform enable working under the thermobaric conditions of the real reservoir. Mimicking real-field scenarios, the recombined live oil composition was used along with recombined associated petroleum gas. During each test, oil was displaced by gas with a minimal flow rate, whereas miscibility was determined based on the analysis of front propagation. The set of experiments was conducted at a temperature of 110 ℃ under

pressures varying from 35 to 42 MPa. In total, five discrete microfluidic displacement tests were successfully performed. Additional tests that involved backfilling the microfluidic chip were done at the same pressure conditions, exhibiting high experimental repeatability. At each pressure point, displacement coefficients were determined based on the processing of experimental videos with subsequent post-analysis. The MMP value of 39.9 MPa was obtained by plotting all the experimentally determined displacement coefficients at different pressures and constructing two linear approximation lines for miscible and immiscible regimes. A comparative analysis of microfluidic and slim-tube approaches showed a relative difference of less than 5%, which proved the validity of the presented method. The proposed methodology has demonstrated its potential for accurately determining the MMP, which would have significant implications for the gas EOR projects in the fields. Each run of microfluidic experiment required less then 10 ml of recombined oil, which was more than ten times less than for an experiment on a slim-tube test. Moreover, a single microfluidic took less than half a day to complete - five times less than for a slim-tube test.

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761

The Wavelength of Viscous-Unstable Displacement in CO2 Sequestration

Authors: Omidreza Amrollahinasab[None]; Holger Ott[1]; Steffen Berg[2]

[1] *Montanuniversität Leoben*

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Carbon sequestration and utilization (CCUS) remains a central strategy for keeping global temperature increases below 1.5° C. Recent research suggests that relevant CO_2 sequestration scenarios where much less viscous CO_2 is injected into permeable subsurface formations to displace more viscous brine could introduce viscous instability.

To assess the impact in terms of storage capacity and plume migration distance, the pressing question is what the dominant wavelength of unstable fingers is and how it depends on key parameters such as rock permeability, fluid viscosity and interfacial tension.

By using Darcy-scale numerical simulations, we find that the finger wavelength scales linearly with interfacial tension and permeability, consistent with the King & Dunayevsky and Yortsos & Hickernell long-wavelength instability findings for immiscible fingering, where mixing in the capillary dispersion zone around the displacement front becomes the counteracting mechanism controlling the wavelength of the maximum unstable growth rate but inconsistent with the much more common Saffman & Taylor description for (short wavelength) immiscible fingering assuming a capillary restoring force.

The resulting finger wavelengths for carbon capture and sequestration (CCS) relevant conditions

range from tens to a hundred meters, while the Saffman & Taylor description drastically underpredicts the wavelength (centimeters or less).
Finger wavelengths at this scale may be a contributing factor to why plume migration was observed to follow the structure of the top seal in CCS field projects and was subject to increased capillary control to a larger extent than initially predicted.

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Poster / 762

Integrated Microstructural Analysis of Rock Samples: Quantifying Porosity and Mineralogy with SEM and Machine Learning

Authors: Mingze Jiang[1]; Eva Wellmann[1]; Joyce Schmatz[1]

[1] *MaP - Microstructure and Pores GmbH*

Corresponding Authors: mingze.jiang@rwth-aachen.de, joyce@m-a-p.expert, eva@m-a-p.expert

Integrating Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), and advanced machine learning techniques like the U-Net model offers new tools and approaches for research in the fields of microstructure analysis and mineralogy. This interdisciplinary approach not only increases the precision of data analysis but also expands the scope of research methodologies.
This study details a methodical approach to the microstructural analysis of rock samples, focusing on the precise quantification of porosity and mineral composition. The process begins with the preparation of rock samples using Broad Ion Beam (BIB) polishing, ensuring optimal surface quality for imaging. The prepared samples are then examined using Scanning Electron Microscopy images, revealing detailed microstructural features.
A significant advancement in our methodology is the use of a pre-trained U-Net model for accurate pore segmentation 1. This machine learning approach efficiently delineates the pore structures within the rock matrix from secondary electron (SE2) images. Subsequently, the study involves analyzing the mineralogical composition of the rock samples. This is achieved through the use of high-resolution backscattered electron (BSE) imaging coupled with low-resolution EDS data. A semi-automatic phase segmentation tool is employed to identify and quantify the different mineral phases present in the rock. This tool incorporates advanced algorithms for pixel-wise image segmentation and labeling, using a decision tree to pinpoint specific minerals 2.
The culmination of this study is the alignment of SE2 and BSE images, enabling the correlation of porosity data with the distinct mineral phases. This innovative technique offers a comprehensive view of how porosity is distributed among various minerals, providing a deeper understanding of the rock's microstructural properties.
This research methodology offers a unique and in-depth perspective on rock microanalysis, with

significant implications for geological research and practical applications across various industries.

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1 Klaver, J., Schmatz, J., Wang, R., et al. Automated Carbonate Reservoir Pore and Fracture Classification by Multiscale Imaging and Deep Learning, 82nd EAGE Annual Conference & Exhibition, Oct 2021, Volume 2021, p.1 –5. 2 Jiang M, Rößler C, Wellmann E, et al. Workflow for high-resolution phase segmentation of cement clinker from combined BSE image and EDX spectral data. Journal of Microscopy, 2022, 286(2): 85-91.

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Poster / 763

Unveiling Microbial Activity in Rock Pores: Tailored Sample Preparation and SEM-EDS Insights

Author: Joyce Schmatz[1]

Co-authors: Eva Wellmann [1]; Mingze Jiang [1]

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Studying the interactions among microbes within rock pores and their impact on mineral phases is essential for comprehending subsurface ecosystems and biogeochemical processes, particularly in the realm of subsurface energy operations. In this paper, we introduce an approach that merges customized sample preparation methods with traditional Scanning Electron Microscopy (SEM) featuring Energy-Dispersive X-ray Spectroscopy (EDS) to both visualize microbes in rock pores and analyze the alterations in mineral phases induced by microbial activity.
Customizing the sample preparation process is crucial to preserving the delicate microbial structures within rock pores. We have devised a protocol that incorporates gentle fixation, embedding, and broad-ion-beam (BIB) polishing to preserve the in-situ arrangement of microbes while facilitating optimal SEM-EDS analysis. This method minimizes sample artifacts, enhancing the accurate representation of microbial structures. Through careful selection of imaging parameters and leveraging SEM imaging, we successfully visualized microbes in their natural habitat, allowing us to observe patterns of microbial colonization, biofilm formation, and interactions with mineral surfaces.
The addition of EDS analysis complements SEM imaging by furnishing elemental composition data at micro- to nanoscale resolutions. Mapping mineral phases and identifying elemental changes induced by microbial activity provided valuable insights into biomineralization processes, dissolution, and precipitation events. Such information is crucial for understanding how microbial communities influence the mineralogical composition of rocks. Our findings highlight the diverse microbial communities residing in rock pores and their intricate impact on mineral phases. Distinct patterns of mineral alteration, including the formation of biominerals and the dissolution of specific phases,

were observed. The integration of tailored sample preparation techniques with conventional SEM-EDS emerges as a straightforward yet potent tool for investigating microbial interactions in rock pores.

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MS04 / 764

Molecular Dynamics Simulations of Porous Illite Clay Surfaces and Particles

Author: Ge Li[1]

Co-authors: Astrid de Wijn [1]; Erika Eiser [1]; Ida-Marie Høyvik [1]; Lu Xia [1]; Rene Tammen [2]

[1] *NTNU and PoreLab*

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Illite clay constitutes the main component of the Norwegian quick clay that is known for its tendency to transform rapidly from a solid to a liquid state under certain pressure.1 Currently the practical method for stabilizing quick clay involves the use of cement and lime, resulting in significant CO2 emissions.2 To explore more environmentally friendly stabilizers, nanoscale theoretical understanding of the mechanical forces between illite particles is essential. The interaction between clay particles depends on the thickness of electrical double layer (EDL) that can be controlled by the types and concentrations of salts.3 In quick clay, a higher salt content results in a thinner EDL and reduced repulsive force. Conversely, if the salt is leached out due to underground water, the EDL thickens, leading to a stronger repulsive force and worse stability. This research primarily focuses on non-equilibrium molecular dynamics simulations involving the direct contact between an illite particle and surface. It aims to elucidate the connections between this interaction and the variations in the EDL resulting from the addition of different salts, such as NaCl, KCl, CsCl, and CaCl2.

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Conference Proceedings:

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Poster / 766

Pore-Type-Dependent microstructures of Shales and Implications on Permeability

Author: Qian Zhang[1]

Co-author: Yanhui Dong

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Pore structure features govern the capacity of gas storage and migration in shales and are highly dependent on the types of pores, i.e., interparticle (InterP) pores, intraparticle (IntraP) pores and organic matter (OM)-hosted pores. However, microstructures and fractal features regarding pore types and their respective contributions to permeability have been rarely addressed. Based on SEM and FIB-SEM imaging, fractal dimensions (Ds) have been determined from both pore size distributions and digital rock to quantify the heterogeneity in pore morphology and spatial textures. Overall, OM-hosted pores are smaller in size and more abundant in quantity, corresponding to a relatively high D, while IntraP pores are mainly isolated and scarce, translating into lower D values. Additionally, crack-like InterP pores with a moderate level of porosity and the D can play a pivotal role in shale seepage potential. A comparison of the estimated permeability among different pore types highlights that the contribution of interconnected OM pores to the overall permeability remains constrained unless they can link neighboring pore clusters, as commonly observed in organo-clay composites. Furthermore, pore morphology and fractal features of shale rocks can exhibit noteworthy variations subjected to sedimentology, mineralogy, diagenesis and OM maturation.

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MS23 / **767**

The Effect of Film Flow on Capillary Pressure Equilibration in Multi-Phase Flow With Disconnected Phase

Authors: Tianyi Li[1]; Dorthe Wildenschild[2]

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Previous studies have demonstrated that curvature-based capillary pressure and transducer-based capillary pressure agrees well for both imbibition and drainage at equilibrium, if only connected fluid interfaces were analyzed. In this study, we further demonstrate that as long as the system reaches equilibration, curvature-based capillary pressure are representative for both connected and disconnected fluid interfaces regardless of whether the system is undergoing imbibition or drainage.

For a water-Soltrol 220 fluid system, we observed that the volume of disconnected nonwetting phase blobs grew during both imbibition and drainage, and surprisingly, growth was faster during drainage than imbibition. We calculated the thickness of the non-wetting phase films using the approach of Chester (1991), and based on this film thickness estimate, we calculated the flow rate of water through a sheet of film, then using the measured change in volume, we estimated the time needed for disconnected phase to equilibrate with the bulk phase via films. The results showed that the time required was well-within the time allowed for equilibration between scans.

This suggest that, due to the limitation in image resolution, some nonwetting phase blobs would be classified as "disconnected", while it appears they may actually be connected through an "invisible" thin film of thickness below the image resolution. This has important implications for how we think about trapping in multi-phase porous medium systems, and the relative importance of flow in films with a thickness below the image resolution in equilibration processes.

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MS06-B / **768**

Experimental Investigation of Illite Clay in Norwegian Quick Clay for Sustainable Ground Stabilization

Author: Rene Tammen[1]

Co-authors: Astrid de Wijn [2]; Erika Eiser [1]; Ge Li [3]; Ida-Marie Høyvik [2]; Lu Xia [2]

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Quick clay is a young geological clay formation and has been formed during the last glacial ice age. Due to the isomorphic substitutions in these phyllo-silicates, their flat surfaces are net negatively charged (1). The Na+ cations which come from the main salt in the marine environment (35g/L) is attracted by the negatively charged surface and neutralizes it. As a result, the particles have a thin diffuse double layer (DDL), leading to flocculation in a "House- of-cards"structure (2,3,4). Due to the isostatic rebound above sea level, fresh water can infuse into the marine deposits, causing salts to leach out. With the loss of cations, the Coulomb forces between the clay platelets increase and overcome the attractive van der Waals forces, and the structure becomes extremely sensitive (5,4). When this structure is disturbed, the clay formation turns into a low-viscosity fluid, and a catastrophic landslide occurs.

To stabilize quick clay, a deep mixing technology with lime and cement is used. Although this technology has been improved over the past decades, it still has a high carbon footprint.
To provide a more sustainable stabilization, our project "Sustainable Stable Ground"investigates the quick clay formation from an atomic scale and upscale to geological scale.

Here, our focus lies in examining the interaction between clay particles through experimental investigation of illite suspensions under different conditions, such as different ionic strength and adding various additives. For our experiments we are using the Tiller-Flotten quick clay from the area around Trondheim, Norway.
Our process involves purifying the clay from the natural ground and characterize the physical- chemical properties using diverse methods such as Scanning Electron Microscopy (SEM) and Elemental Analysis (EDS). With the objective of identifying potentially sustainable stabilizers, we create different suspensions with diverse (sustainable) additives, allowing for a long-term observation of the clay-rich ground.

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MS23 / 769

Visualizing Mass Transfer Across Fluid-Fluid Interfaces

Author: Anna Herring[1]

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When a nonwetting fluid is forced to flow through an otherwise water-saturated porous solid medium (e.g. as occurs in geologic CO_2 sequestration and underground hydrogen storage projects), the movement and ultimate fate of that nonwetting phase is dictated by a range of physio-chemical interactions; including trapping within pore spaces due to capillarity, mobilization via viscous or buoyant forcing, and dissolution and subsequent flow within the aqueous phase. Previous studies have constrained these transport processes, often using the explicit assumption that capillary trapping (or mobilization) and dissolution are distinct mechanisms, occurring on disjoint length and time scales. However, our recent experiments 1 suggest that there exists a strong coupling of these processes: dissolution shrinks ganglia and changes bubble morphologies; and it may also induce a concentration gradient near the ganglion interface that locally decreases the fluid-fluid interfacial tension. We observed that these impacts frequently destabilized previously trapped ganglia, ultimately inducing buoyant displacement upwards 1.

To further explore this coupled transport behavior, we have designed and deployed a novel experimental protocol which allows us to visualize dissolution mass transfer across fluid-fluid interfaces at the pore-scale. Here, we present preliminary results for CO_2 gas bubbles dissolving within a 3D packing of spherical beads, refractive-index matched to water. The water phase is doped with pH-sensitive fluorescent indicator. Once a CO_2 bubble is introduced and capillary trapped within the system, we apply Planar Laser Induced Fluorescence (PLIF) to visualize the pore-scale evolution of aqueous pH (i.e., aqueous CO_2 concentration) during the dissolution process. Our results demonstrate the variability of dissolved gas concentration at the pore-scale, and the influence of the fluid-fluid interface on the dissolution process. This study thus builds on the foundational work of Prof. Dorthe Wildenschild: focusing on interfacial dynamics of multiphase systems, and highlighting potential impacts to the long-term behavior of capillary trapped ganglia.

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1 Huang, R., Herring, A. L., & Sheppard, A. (2023). Investigation of supercritical CO2 mass transfer in porous media using X-ray micro-computed tomography. Advances in Water Resources, 171, 104338. https://doi.org/10.1016/j.advwatres.2022.104338

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MS11 / 770

Approach for void space reconstruction on a microchip based on the lithological and mineralogical data

Author: Margarita Latypova[1]

Co-authors: Alexey Cheremisin [2]; Dmitrii Pereponov [2]; Eduard Batyrshin [3]; Evgeny Shilov [2]; Igor Maryasev [4]; Michael Tarkhov [5]; Roman Mukhin [4]; Timur Nigmatullin [3]; Vitaly Kazaku [2]; Vladimir Kosorukov [6]; Vladimir Shtinov [3]; Igor Samsonov [7]

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Tight gas reservoirs are the subject of interest to many researchers because of the large oil and gas deposits concentrated in them. These low porosity and permeability sandstone reservoirs are widespread worldwide. Enhanced oil recovery methods are widely used in the industrial development of such deposits. These methods require numerous preliminary coreflooding experiments on rock samples, which are expensive and, in many cases, impossible to perform, having only one sample because coreflooding tests almost always consist of multiple steps.

Therefore, we assume replacing the structure of a real core void space with a similar artificially created geometry inside a silicon microfluidic chip that can be used many times in flooding experiments without damaging the core-prototype sample. However, it is crucial to take into account such parameters as wettability, pore size, pore distribution, length, width, and tortuosity of pore channels, et al. A special role in studying such parameters is always assigned to the relationship between the lithological and mineralogical characteristics of the rock with its structure of the void space according to microtomography (MCT) data.

The current research aims to identify features of the mineral matrix of studied tight gas sandstone reservoirs, which most intensively influenced the void space structure. The study represents preliminary work before conducting flooding tests on microfluidic chips with heterogeneous wettability to limit water inflow. We have used such methods as MCT data, lithological study rocks in cross-sections, X-ray diffraction analysis, grain-size analysis, and mineralogical composition by scanning electronic microscopy. As a result of current studies, we have determined that all rocks with different permeabilities have almost the same mineralogical composition. The difference is that the mineral matrix of rocks with low permeability has a higher content of secondary calcite minerals. Most of the macropores (>2 μm) identified by MCT data were caused by secondary leaching of plagioclases. Most of the microporosity (<2 μm) is associated with clayey chlorite cement. Primary porosity is almost entirely replaced by secondary silicification due to the intense secondary transformation of sandstones.

The second part of the current study was dedicated to the creation of void space structures in microfluidic chips using the complex of lithological, mineralogical, and, to a greater extent, MC data. We have developed a new method of creating an artificial pore structure of microfluidic chips that retains a large number of properties of the original core when moving from 3D to 2D structures. Moreover, using mineralogical data, we developed a model of heterogeneous wettability of void space in microfluidic chips to repeat the wettability in natural reservoir rocks. We assumed the model with hydrophobic macropore space and hydrophilic micropores because of the capillarity forces that retain water in smaller pores.

In conclusion, current research gave us complete information about mineralogy and the void space

geometry of the core samples from the studied tight gas reservoirs. With these data, we could extrapolate future results of microfluidic tests to nearby tight gas sandstones with the same mineralogical composition.

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MS01 / **772**

Methods for Hydrogen Storage Characterization in Porous Substrates

Author: Vladimir Alvarado[1]

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Hydrogen energy has been a subject of increasing interest over the past decade. The use of hydrogen for energy storage allows for a clean energy carrier that produces only water and heat after oxidation. Focus has been hydrogen storage, which demands abundant and safe storage volumes. Similar to the carbon dioxide storage campaign, subsurface formations offer large pore volumes for gas storage, but characterizing porous substrates for this purpose is still in development. Depleted oil reservoirs, salt dome caverns, and aquifers are prime subsurface candidates for this purpose. There are associated issues with the injection of large volumes of the gas into these formations such as unfavorable chemical reactions, leakage through the cap rock, and large capital expenses associated with suitable surface injection equipment. This research aims at testing our ability to estimate adsorption capacity in synthetic or natural porous systems. To this end, materials were first characterized via low-pressure adsorption isotherm analysis. Secondly, low-pressure nitrogen adsorption results were compared to nitrogen and hydrogen high-pressure adsorption isotherms to determine if surface area analysis suffices to estimate storage potential for hydrogen. Additionally, nuclear magnetic resonance (NMR), first in its non-spectroscopic mode, namely Time Domain NMR (TD-NMR), and subsequently in its spectroscopic mode, using a high-field NMR spectrometer, was used to analyze hydrogen adsorbed in porous media. In this sense, we developed TD-NMR protocols that enabled capturing data at relatively high pressure (up to 3000 psi) using a custom-designed NMR tube in which the gas pressured was controlled with a pump. A similar setup was used on a Bruker Biospin NMR spectrometer. Results show that low-pressure nitrogen adsorption isotherms provide insufficient guidance to understand the hydrogen adsorption response at high pressure, which likely reflect the fact that surface area is at best an incomplete characterization method for this purpose. TD-NMR transverse relaxation time (T2) distribution shows some sensitivity to hydrogen adsorption in porous media at high pressure, which indicates the potential of this technique to characterize hydrogen storage. High-field NMR, while being a more complex method, sheds light on hydrogen behavior in porous media that complements the other two sources of information.

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MS13 / **775**

Water effect on oil adsorption and configuration in nano mineral pore

Author: Hang Jiang[1]

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Sedimentary rock is wet in situ and generally occurs at depths in the subsurface where pores are saturated with water and hydrocarbons. The competitive adsorption of water and oil in nanopores of shales is believed to influence the dynamic configurations of fluids, and therefore their wetting and displacement behaviors and ultimately oil production. But its nature is poorly understood due to nano-confinement induced challenges in performing both physical and numerical experiments. In this study, the effects of water as a competitive adsorbate on the adsorption of n-heneicosane in Na-montmorillonite (MMT) and illite slit nanopores, with a 5-nm aperture, are systematically investigated and elucidated using molecular dynamics (MD) simulations, under realistic conditions. For each pore, water and oil molecules at selective concentrations (100%, 0), (25%, 75%), (50%, 50%), (75%, 25%) and (0%, 100%) are packed randomly into the pore at the same time and then are geometrically optimized before a stable configuration in NPT ensemble is obtained to perform MD simulation runs for estimating the density distributions for both phases.

The results show that the water molecules are the preferred adsorbate to both minerals and form an apparent wetting layer when both water and oil molecules enter the pore at the same time. These appear relatively more distinctive for the MMT than illite pores, in particular, at low water concentrations. When the oil molecules enter a pore earlier than the water molecules, or vice versa, the early-entering molecules are found to impede the late-entering ones from being absorbed onto the pore wall of MMT. The molecules, which are adsorbed to the pore wall, seem to adsorb the molecules of the other phase in the pores, to yield a smooth transition zone between adsorbed and free phases. The water molecules are found to disperse into the oil molecules, and when the water concentration is high enough, the former form bridges from one wall to another, and a film on the mineral surface. At 75% oil concentration, the oil molecules are found to be adsorbed on the wall of both MMT and illite pores but not appears as a flat film. This study offers new insight into the nature of the competitive adsorption and discusses its impact on phase configurations in pores and wetting behaviors.

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776

Impact of nanoconfinement on the pressure dependence of elastic moduli

Authors: Klaus Schappert[1]; Rolf Pelster[1]

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Previous experimental and theoretical studies revealed that the confinement of a substance in nanopores causes an enhancement of its elastic moduli [1,2]. For example, using ultrasonic measurements we have shown that the longitudinal modulus β_{ads} of confined liquid adsorbates (noble gases, nitrogen) is higher than that of the corresponding liquid bulk substances (see, e.g., Ref. [3]). The strength of this enhancement is related to the interaction between adsorbate and pore surface and consequently it can also depend on temperature [3].
Apart from the values of the elastic moduli it is also of interest whether their pressure dependence deviates from bulk behavior. In fact, curved liquid-vapor menisci of the adsorbate in the nanopores cause a high negative Laplace pressure, p_L, that can be varied [4]. We determine the dependence of adsorbates'longitudinal moduli on this Laplace pressure, $d\beta_{ads}/dp_L$, at various temperatures. Based on our experimental data we discuss the impact of nanoconfinement, i.e., we compare $d\beta_{ads}/dp_L$ and its temperature dependence with the pressure dependence for the bulk substances, $d\beta_{bulk}/dp\,(T)$.

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1 Christopher D. Dobrzanski, Boris Gurevich, and Gennady Y. Gor, Elastic properties of confined fluids: From molecular modeling to ultrasonic experiments on porous solids, Appl. Phys. Rev. 8, 021317 (2021). 2 Klaus Schappert and Rolf Pelster, Elasticity and Phase Behavior of Fluids in Nanoporous Media, pp. 259-304, in Soft Matter and Biomaterials on the Nanoscale, Vol. 1, Patrick Huber (Ed.), World Scientific (2020). [3] Klaus Schappert and Rolf Pelster, Distinct Enhancement of the Longitudinal Modulus of

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Poster / **777**

Microfluidic visualization of asphaltene deposition under high temperature

Authors: Dmitrii Pereponov[1]; Evgeny Shilov[1]

Co-authors: Michael Tarkhov [2]; Tagir Karamov [3]; Alexander Rykov [2]; Ivan Filippov [2]; Natalya Lesina [4]; Evgeny Popov ; Pavel Grishin [3]; Alexey Cheremisin [1]

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The goal of this study lay in the evaluation of the asphaltene deposition on the artificial 2D porous structure of the carbonate rock using high-pressure and high-temperature (HPHT) microfluidic technology. Such technology was utilized to evaluate the behavior of heavy oil quickly and effectively under reservoir conditions, on par with traditional tests. Our workflow started with the designing of microfluidic chip structure. Based on computed tomography data, a unified geometry of the porous space was developed, with pores and pore throats close to the target formation. The resulting design was realized as a silicon-glass microchip that can withstand high temperatures (up to 350℃) close to the formation during steam injection. In the first step, the dead heavy oil was injected into the whole microfluidic system at the ramped temperature. Later, high-viscous oil was displaced by the solvent, and then the precipitated heavy fractions were analyzed with microscopy. The microfluidic experiments were conducted under four different temperature conditions. At stages of 50 and 110℃, during displacement of heavy oil with n-heptane, there was no attenuation of filtration or precipitation of heavy fractions. The permeability of the microfluidic chip was found to decrease as deposits formed in the filtration channels during the third stage of the experiment at 170℃. The deposition of heavy fractions was confirmed by visual inspection of the microfluidic channels and analysis of the deposited material using scanning electron microscopy (SEM). The nature of a deposition was established by comparing the image in white and fluorescent light. Precipitation of an organic nature (asphaltenes) fluoresced, while deposits that did not fluoresce were mechanical impurities. For the last test, a new clean microchip was utilized, where displacement at 300 ℃ resulted in a similar blockage of the channels by asphaltenes and fine mechanical impurities (particle size less than 3 microns). Overall, the results suggest that temperature plays a crucial role in asphaltene deposition for heavy oil. These findings have valuable implications, since asphaltene deposition is a significant problem during oil production and transportation. The conducted experiment has demonstrated its effectiveness for studying the behavior of high-viscous oil at elevated temperatures using HPHT microfluidic technology. Further studies are needed to investigate the underlying mechanisms of asphaltene deposition, develop effective strategies to mitigate this problem, and conduct the sensitivity analysis to bring new insights to the effective heavy oil reservoir development.

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MS07 / 778

Quantifying Uncertainty in the Predictive Power of Multi-Scale Pore-Scale Modeling of Complex Microporous Media

Author: Sajjad Foroughi[1]

Co-authors: Branko Bijeljic [2]; Martin Blunt [3]

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In this study, we explore the complex behavior of multiphase flows, exemplified by CO2 movement in underground reservoirs, within the context of heterogeneous porous media such as carbonate rocks. These materials display a wide range of pore sizes, posing significant challenges for imaging-based models due to the inherent trade-off between image size and resolution. Often, finer details are sacrificed in order to capture a comprehensive view of the pore structure in carbonates.
Addressing this issue, our approach involves the detailed analysis of sub-resolution porosity within X-ray images. We employ differential imaging techniques to highlight the differences between dry scans and scans of rocks saturated with 30 wt% KI brine. Building on this analysis, we have devised a novel workflow that integrates this sub-resolution porosity into a network model, using elements we refer to as 'micro-links.' These are based on Darcy's law and link each grain voxel, identified with sub-resolution porosity, to the nearest resolved pores through an automated dilation process.
Our modeling framework extends to both single-phase and multiphase flow simulations, incorporating these micro-links and corresponding empirical models. We have fine-tuned these models to ensure that our predictions regarding effective permeability, formation factor, and drainage capillary pressure are in line with experimental observations. The calibrated model is further employed to predict relative permeability, with a particular focus on quantifying the associated uncertainties. Moreover, we aim to thoroughly investigate and quantify how microporosity influences fluid distribution and phase behavior within these porous media. This quantification of uncertainty is pivotal in evaluating our model's predictive accuracy and enhancing our understanding of multiphase flow dynamics.

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MS01 / **780**

Ostwald Ripening Leads to Less Hysteresis during Hydrogen Injection and Withdrawal: A Pore-Scale Imaging Study

Author: Sepideh Goodarzi[1]

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Utilising depleted hydrocarbon reservoirs or aquifers for hydrogen storage shows promise due to their substantial storage capacity. Efficiently managing hydrogen storage requires careful consideration of hysteresis across multiple cycles. Hydrogen experiences both injection and production, usually on a seasonal basis, impacting both hydrogen recovery and pore space entrapment. Our study investigates the capillary pressure hysteresis induced by this cyclic injection and withdrawal process, employing X-ray tomography. This exploration holds potential for optimising subterranean hydrogen storage systems. Conducting experiments under dynamic conditions, we analysed gas and water distribution within distinct pore space geometries during drainage and imbibition cycles. We injected the gas phase into 6 cm long samples of Bentheimer sandstone at ambient temperature and 8 MPa pore pressure, followed by three water flooding cycles. Varied gas saturation levels—high, medium, and low—were achieved while maintaining a constant brine flow rate, allowing a comprehensive exploration of distribution dynamics. Throughout these cycles, our observations unveiled intriguing phenomena: (I) capillary pressure hysteresis and (ii) hydrogen migration through Ostwald ripening. Contrary to conventional models, our results suggest the possibility of surpassing the presumed residual gas saturation through further injection and withdrawal, challenging the assumed gas recovery limit. To further understand these phenomena, we analysed interfacial curvature and area, conducted wettability assessments, and performed pore occupancy analysis. These insights offer a pore-scale understanding of hydrogen storage dynamics, providing crucial image-based data essential for modelling multiphase flow properties in reservoir-scale simulations.

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Poster / 781

Neural Operator Predictions of Electrical Properties in Porous Media

Author: Bernard Chang[1]

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The characterization of electrical transport properties through porous media is commonly used for reservoir formation evaluation, groundwater management, mineral exploration, and carbon capture and storage (CCUS) monitoring. We discuss image-based characterization and prediction of a range of transport properties including, but not limited to, flow/momentum transport, mass transport as well as electrical properties, often in the presence of multiple fluid phases. We then present novel data science methods and their impacts on prediction speed and accuracy. The data used in this work is openly available as part of a benchmark dataset that includes complete geometric characterization and simulations hosted on Digital Rocks Portal1.

Deep learning (DL) has emerged to be a powerful tool for modeling these transport properties while reducing computation time by several orders of magnitude. Previously, we have applied convolutional neural networks (CNNs) to predict the electric potential field given a segmented x-ray microtomographic image. We found that the set of input features used to predict momentum and mass transport properties did not translate well to electrical transport and had to be redesigned. We further found that because classical DL networks (including CNNs) typically provide a mapping between Euclidean spaces (e.g. image vector-to-scalar quantity, image vector-to-image vector, etc.), they effectively only learning a single instance of the governing equation. If the discretization of the partial differential equation (PDE) changes, the model needs to be retrained or can otherwise lead to issues when applying the model to new domains. Here, we present new work on overcoming that limitation by training neural operators.

Neural operators are a new subclass of scientific machine learning in which data-driven models learn mappings between function spaces, thus learning entire families of PDEs. Here, we apply a Fourier neural operator network to predict the electric potential through a 3D porous medium and contrast them to classical convolutional neural networks (CNNs). The results show improved accuracy over previously trained CNNs, particularly when introducing new types of porous media. Further, we recognize that training a neural operator network typically requires large amounts of high-fidelity data, and despite the existence of open data portals, such as Digital Rocks Portal, this is nevertheless a bottleneck. To address this, we explore the development of a multiscale neural operator network. We expect that the initial time-intensive training will be compensated by its ability to generalize to new parameterizations and other transport problems in porous media.

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MS09 / 782

Volume of Fluid based study of the three phase dynamic contact line in wetting of the nanometric rough micro-channels

Authors: Tianyang Han[1]; Yash Kulkarni[1]; Tomas Fullana[None]; Stephane Zaleski[2]; Stephane Popinet[1]

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The precise representation of molecular motion near the three-phase dynamic contact line remains a significant research challenge 1, with substantial practical implications 2. We investigate the two-phase flow in a pressure driven micro channel (width ~ 1μm - 10μm) having a nanometric surface roughness. The two phases are separated by an interfacial layer with surface tension, that meets the moving pipe wall, hence, a three phase dynamic contact line is formed. Numerical simulations are conducted by solving the 2D two-phase Navier-Stokes equation using the Basilisk flow solver. The Volume-of-Fluid method is employed to capture the interface, and the surface tension force is computed using the Continuous Surface Force method. Additionally, curvature calculation is done using height functions. To address the influence of surface roughness, we develop a hybrid Volume-of-Fluid coupled embedded boundary solver. This hybrid solver enables the imposition of a contact angle on arbitrarily shaped solids. We explore scenarios where (a) surface roughness exhibits periodicity, (b) the surface is scratched or bumped with rough patches, and (c) surface heterogeneities are present. The study quantitatively demonstrates the emergence of stick-slip behavior in these scenarios allowing us to verify the thesis of Hocking [3] and Jansons [4]. Our findings serve as a prerequisite for full pore-scale Direct Numerical Simulation (DNS), ensuring a high-fidelity representation of dynamic wetting phenomena in porous media.

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[3] Hocking LM. A moving fluid interface on a rough surface. Journal of Fluid Mechanics. 1976;76(4):801-817. doi:10.1017/S0022112076000906

[4] Jansons KM. Moving contact lines on a two-dimensional rough surface. Journal of Fluid Mechanics. 1985;154:1-28. doi:10.1017/S0022112085001392

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MS23 / 783

Harnessing the power of microstructure imaging through open data, software and education: past, present and future of Digital Rocks Portal

Author: Masa Prodanovic[1]

Co-authors: Bernard Chang [1]; Cinar Turhan [1]; Ali Mohamed [1]; Maria Esteva [1]; Richard Ketcham [1]; James McClure [2]

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Modern 3D imaging provides a window to the microstructure of soil and rocks, and recent advances in experiments, simulation and data science can improve our understanding of how these materials influence the world around us. The Digital Rocks Portal (DRP, https://www.digitalrocksportal.org) is the first platform of its kind for porous media images' management. It has an impressive collection of experimentally captured multiphase x-ray microtomography configurations. The open science materials surrounding the platform follow Dr. Wildenschild's vision closely.

History of the portal: It is less known is that the precursor of the portal was inspired by Dr. Wildenschild. Drs. Wildenschild, Peszynska and Prodanovic recognized in 2008 and had many discussions on the need for validation and comparison of experimental, theoretical and numerical approaches. We organized a Wiki page Pore Scale Benchmark project 2009-11 (now deprecated) with links and descriptions of related data and code. The data required dedicated storage and support, however, beyond what a wiki page is meant to provide: open science is not free, and requires resources. This project was a pre-cursor of Digital Rocks Portal which went live in 2015 with the help of two National Science Foundation (NSF) grants and you can find many of Prof Wildenschild's datasets on DRP.

History of short courses: Prof. Wildenschild is a visionary educator. Once upon a time in 2010, and despite an explosion of available x-ray microtomography and SEM images providing insight into rock microstructure, structured courses on image-based quantification within relevant graduate programs were mostly unavailable. Prof. Prodanovic approached Prof. Wildenschild and Prof. Sheppard (Australian National University) with an idea to teach a short course on image analysis in porous media in 2010. We together created the first short course and workshop in July 2011 at The University of Texas at Austin. The course was repeated in 2013 at InterPore Society Annual Conference 2013 and was one of the first InterPore short courses. We all separately developed full length graduate courses at our home institutions, followed by the courses taught connected to both Digital Rocks Portal platform and InterPore Academy.

Present: DRP has an active community that publishes and reuses the data, most recently in multiple machine learning applications. We have 155+ published datasets (projects) cited in 210+ published papers and are expanding the scope to curate energy storage materials. The platform has been rebuilt on the new infrastructure in Texas Advanced Computing Center from Jan to May 2024.

Future: We present the new digital porous media open source software tools related to the portal. Those include: gray-scale image processing, and visualization; an automatic scale-independent method for classifying rock heterogeneity of binarized images; (2) velocity field analysis and visualization, (3) flow simulation and (4) machine/deep learning. We are thus close to having an open science environment for cross-validation and data-driven upscaling of microstructure properties in subsurface engineering, material science and geosciences.

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Poster / 784

Model formulation of fluid flow in phase domain for fracturing-shut in-flowback-production process in tight oil reservoirs

Author: Zhixue Zheng[1]

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Multistage hydraulic fracture stimulation is commonly used with horizontal well technology as one of key technologies for the economical and effective development of unconventional reservoirs such as tight oil. The applicable method of numerical simulation will provide effective modeling tools for quantitative studies of tight oil reservoir dynamics and performance, fractures and their effects on oil production, well and stimulation design, and optimal production schedules in the field. The field shows that the flowback rate of fracturing fluid in tight oil reservoir is related to increasing and stabilizing production, and the technology of fracturing, shut in and production has achieved a positive effect on increasing production. However, there are few standardized and effective numerical modeling approaches available for guidance. Based on the summary and analysis of recent research results on the imbibition and flowback of fracturing fluid in tight reservoirs, a novel numerical model of fluid flow for fracturing, shut in, flowback, and production process in tight oil reservoirs is proposed considering the mechanism of spontaneous imbibition, hysteresis effects of capillary pressure and relative permeability, osmotic pressure, stress sensitivity, fluid compression effect in fractures and water-rock interaction. In this model, the multi-scaled fracture system of tight oil reservoirs is described as a set of subdomains and handled by a multi-continuum conceptual model. To model the effect of fluid compression, the pores and fractures of tight reservoir are classified and described according to the different compressibility of tight oil and fracturing fluid. When considering the stress sensitivity of different types of pores and fractures, the effects of fluid distribution difference and fluid compressibility are considered. The model in this paper can describe the fluids flow in pores and fractures in a more detailed and accurate manner, and has certain reference value for understanding the mechanisms of fracturing fluid imbibition and retention, and enhancing tight oil recovery.

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MS15 / 785

Data Quality Assurance Metrics for Federated Machine Learning

Author: Bernard Chang[1]

Co-authors: Cinar Turhan [1]; Ali Mohamed [1]; Maria Esteva [1]; Masa Prodanovic [1]

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Machine/deep learning (ML/DL) have emerged as powerful tools for driving science innovation. These methods tend to be data hungry, with large volumes that are not likely to be collocated. Further, industry or professional companies typically have a vested interest in keeping their data private. Recent work has shown the viability of federated learning (FL), a ML /DL framework where multiple groups (called clients) collaboratively train a single model without exchanging locally stored, private data. We apply this framework to a problem common in reservoir engineering and digital rocks physics: we use a convolutional neural network with the specific task of predicting the flow velocity field through a porous sample using its segmented x-ray microtomography image as input. The results are nevertheless applicable to any task with spatial data stored across multiple locations participating in training the same model.

As with any typical DL workflow, the quality of the training data plays a key role in the prediction accuracy and the generalizability of a network model. Additionally, the interest in enabling the reusability of these models is guided by the findable, accessible, interoperable, and reusable (FAIR) principles. In the context of FL, the assurance that each client provides quality and representative training data that adhere to the FAIR principles has proven challenging because the data and its metadata remain private.

Here, we first explore how differences in local data can affect prediction behavior once individual models are aggregated. We then propose several preprocessing metrics that can be quickly computed and shared with the central server to assure the quality of the training set but without ability to infer the entire dataset from them. For our specific task of predicting a flow field, we employ common techniques of quantifying pore geometries based on their images. These include, but are not limited to, pore space morphological and topological descriptors, heterogeneity characterization, representativeness quantification, and resolution checks using morphological drainage.

We validate our trained models to test that the proposed metrics properly capture the representativeness of the new training data while still providing sufficient diversity to further the model's learning. The scope of this work is to show that a set of quality assurance metrics enables model reuse under FAIR principles while maintaining clients'data privacy during FL. In a broader context, these metrics are also useful for preprocessing classical machine learning training data and in developing constitutive relationships between complex pore geometries and transport properties. Last but not the least, we discuss how we apply this framework with two industry partners.

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MS01 / **788**

Quantifying the multiphase CO2-brine transport in basaltic rocks

Authors: Jianwei Tian[1]; Yuechao Zhao[2]

Co-authors: Bohyun Hwang [3]; Adedapo Awolayo [1]; Benjamin M. Tutolo [3]

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Amid intensified global efforts to mitigate climate change, carbon mineralization in basaltic formations has emerged as a more prominent, secure, and permanent storage solution for anthropogenic CO2. When CO2 is injected into basaltic rocks, displacing the in-situ pore fluid, the volume of displaced fluid and, consequently, the injected gas depends on the interplay between relative permeability, capillary pressure, and fluid saturation. However, characteristic flow curves specific to basaltic rocks are limited, emphasizing the need for a deep understanding of this multiphase transport behavior to design effective carbon storage systems. Hence, this study addresses this critical aspect by employing the Lattice Boltzmann Method (LBM) on X-ray computed tomography (XRCT) scans of select basaltic rock samples, capturing the complex internal structures of the basalt. These acquired images are reconstructed into digital models that represent the physical characteristics of the basaltic rocks. We utilized these digital models and LBM, based on the sophisticated Shan-Chen framework to compute key transport properties, including permeability, relative permeability, and capillary pressure. This model enables us to accurately simulate the intricate interactions and dynamics of CO2 transport within basalt under varying temperature and pressure conditions. The comparison of the LBM computational results with the limited experimental data revealed a high degree of correlation, thereby validating the accuracy of our simulations. The strong agreement not only attests to the reliability of LBM in the simulation of geological processes but also reinforces our capability to accurately predict CO2 storage in basalt, further affirming its feasibility as an effective carbon sequestration strategy. Overall, our findings provide valuable insights into the dynamics of CO2 storage in basaltic formations, offering a robust foundation for ongoing efforts and future research that will enhance our ability to combat climate change.

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MS08 / 789

Quantifying dissolution dynamics in porous media using a spatial flow focusing profile

Authors: Tomasz Szawełło[1]; Jeffrey D. Hyman[2]; Peter K. Kang[3]; Piotr Szymczak[1]

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Dissolution processes in porous media produce a diverse range of patterns, depending on the relations between flow, diffusion, and reaction rates. Determining the dissolution regimes is critical for controlling contaminant migration, preventing CO2 leakage during geological carbon sequestration, or assessing the long-term stability of hydraulic structures. In all of these cases, the emergence of highly efficient flow paths within rock can dramatically alter its transport properties. To distinguish between these regimes, we analyze a spatial flow focusing profile based on the focusing index developed by Jang (2011). We segment the medium into cross sections along the flow direction and calculate the flow focusing index for each of them. Consequently, we obtain a profile which is a function of distance from the inlet. Through the analysis of this profile and its temporal changes, we observe various types of evolution, such as a front of increased flow focusing progressing from the inlet in the wormholing regime or a decrease in focusing along the entire medium in the uniform regime.

We employ this measure in numerical simulations of a dissolving porous medium using a pore-network model. In this approach, we treat the porous medium as a system of interconnected pipes (Budek, 2012) with the diameter of each segment increasing in proportion to the local reactant consumption. By modifying flow and reaction rates in the simulations, we obtain a phase space diagram displaying a variety of dissolution patterns, which we characterize using our quantitative flow focusing measure. Through this analysis, we identify the elusive channeling regime (Menke, 2023). To generalize our findings, we investigate the impact of network heterogeneity on the emerging flow patterns by varying its magnitude and spatial correlation. The findings elucidate the key parameters that determine the dissolution regimes.

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MS01 / **790**

Evaluating the impact of Hysteresis and Heterogeneity on Hydrogen Storage Performance in Saline Aquifers

Author: Abdolali Mosallanezhad[1]

Co-authors: Amir Jahanbakhsh [2]; John M. Andresen [2]; M. Mercedes Maroto-Valer [2]

[1] *Researcher*

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The imperative to achieve net zero carbon emissions by 2050, aligned with global efforts to limit temperature rise, emphasizes the urgent shift to low-carbon energy sources. Hydrogen is identified as a key player in global decarbonisation however, concerns about the efficiency of hydrogen storage accompany its expanding production. This study investigates underground geological hydrogen storage in saline aquifers, emphasizing the impact of reservoir heterogeneity, flow function hysteresis, and injection/production flow rates on storage efficiency. The results show that hysteresis plays a crucial role in affecting storage efficiency, leading to significant entrapment and a lower recovery factor in initial production cycles. Reservoir heterogeneity leads to non-uniform gas movement in heterogeneous systems and as a result, the efficiency of hydrogen storage is greatly compromised. In addition, the optimal selection of production flow rates presents a challenge in balancing hydrogen recovery and water management. The study highlights the need for customized approaches, emphasizing the importance of aligning flow rates with specific reservoir characteristics for efficient large-scale hydrogen storage.

A set of simulations was conducted to investigate the influence of relative permeability hysteresis, injection/production rates, and reservoir heterogeneity (permeability) on large-scale hydrogen storage performance. The spatial continuity was established as omni-directional in the heterogeneous model and the simulation was conducted in a two-dimensional cartesian system (Figure 1). Both injectors and producers were controlled by the flow rate at reservoir conditions (0.015 PV/day), assuming the fracturing pressure would not be exceeded. The model's end simulated a large aquifer as a spill point, ensuring sufficient volume for input or output to maintain well flow rates in the gas injection and production cycles. The simulation was designed to terminate as soon as the gas reaches the spill point.

Both the homogeneous and omni-directional models exhibited similarities and differences in their hydrogen injection and production behaviour. The homogeneous system, with a consistent injection rate of 6.01305 m3/day, showed higher primary production recovery (72.56%) compared to the omni-directional system (56.60%), where high permeability in specific blocks led to rapid hydrogen advancement and more hydrogen trapping during production cycles. The second injection cycle demonstrated comparable trends in recovery factors for both systems, with the heterogeneous system achieving a slightly higher final recovery of secondary production (97.1%) compared to the omni-directional system (94%). In both systems, by decreasing the gas injection and production rates the final recovery of primary and secondary production was lowered.

Lowering the production flow rate consistently reduces the gas-water ratio in both models due to the decreased mobility difference between hydrogen and water. In the heterogeneous model, since water was displaced unevenly throughout the system (viscous fingering), the waterfront progressed

faster towards the well during the production cycle. As shown in Figure 2, the waterfront eventually reaches the production well, causing a significant reduction in the gas-water ratio, particularly in the second production cycle since a smaller amount of hydrogen was injected during the second injection cycle. This dynamic transition holds substantial implications for storage operation efficiency and becomes a pivotal factor in operational decision-making.

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1 Abdellatif, M., Hashemi, M. and Azizmohammadi, S., 2023. Large-scale underground hydrogen storage: Integrated modeling of reservoir-wellbore system. International Journal of Hydrogen Energy, 48(50): 19160-19171. https://doi.org/10.1016/j.ijhydene.2023.01.227 2 Hashemi, L., Blunt, M. and Hajibeygi, H., 2021. Pore-scale modelling and sensitivity analyses of hydrogen-brine multiphase flow in geological porous media. Scientific Reports, 11(1): 8348. https://doi.org/10.1038/s41598-021-87490-7 [3] Heinemann, N., Alcalde, J., Miocic, J.M., Hangx, S.J.T., Kallmeyer, J., Ostertag-Henning, C., Hassanpouryouzband, A., Thaysen, E.M., Strobel, G.J., Schmidt-Hattenberger, C., Edlmann, K., Wilkinson, M., Bentham, M., Stuart Haszeldine, R., Carbonell, R. and Rudloff, A., 2021. Enabling large-scale hydrogen storage in porous media –the scientific challenges. Energy & Environmental Science, 14(2): 853-864. https://doi.org/10.1039/D0EE03536J [4] Jahanbakhsh, A., Louis Potapov-Crighton, A., Mosallanezhad, A., Tohidi Kaloorazi, N. and Maroto-Valer, M.M., 2024. Underground hydrogen storage: A UK perspective. Renewable and Sustainable Energy Reviews, 189: 114001. https://doi.org/10.1016/j.rser.2023.114001 [5] Rezaei, A., Hassanpouryouzband, A., Molnar, I., Derikvand, Z., Haszeldine, R.S. and Edlmann, K., 2022. Relative Permeability of Hydrogen and Aqueouss Brines in Sandstones and Carbonates at Reservoir Conditions. Geophysical Research Letters, 49(12): e2022GL099433. https://doi.org/10.1029/2022GL099433 [6] Yekta, A.E., Manceau, J.C., Gaboreau, S., Pichavant, M. and Audigane, P., 2018. Determination of Hydrogen–Water Relative Permeability and Capillary Pressure in Sandstone: Application to Underground Hydrogen Injection in Sedimentary Formations. Transport in Porous Media, 122(2): 333-356. https://doi.org/10.1007/s11242-018-1004-7

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MS11 / 791

3D microfluidic investigation of crystallization behavior in porous media for carbon storage application

Authors: Rosalie Krasnoff[1]; Shaina Kelly[1]; Tianxiao Shen[1]

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We investigate the impact of multiphase fluid transport on nucleation and crystallization (precipitation) reactions under pore confinement and the influence of that behavior on permeability and accessible pore space in porous media. Experiments at the intersection of geochemistry and microfluidics have the potential to enable a step change in understanding CO2 storage and mineralization mechanisms by investigating the influence of transport on mineralization rates reported from batch reactor

experiments. To study precipitation of silicate and carbonate minerals in mafic/ultramafic formations for carbon storage applications, we create models of 3D unconsolidated or sintered glass bead "grains"in glass tubes and planar cells with varied reactive inclusion "grains"of (1) mafic/ultramafic minerals including MgO, brucite, and olivine and/or (2) water-soluble seed crystals (e.g., sodium chloride, sodium acetate, copper sulfate) that are mounted in a microfluidic setup. The latter form from supersaturated brines at faster rates than geologic crystals and are used as mineralization proxies to explore crystallization dynamics in a lab microfluidic setting on a reasonable timescale. Mineralization reactions of mafic/ultramafic inclusions are slower, in part because gaseous CO2 must dissolve into the brine and the minerals must dissolve to release ions before the crystal formation can proceed. The microfluidic devices are pre-saturated with a brine of the necessary ionic concentration to promote crystallization. Then, either air or CO2 gas is injected depending on the desired reaction. This multiphase flow produces liquid-gas interfaces that influence crystallization. Flow dynamics and the habits of crystal nucleation and growth under pore-confinement in these engineered porous media are captured with time-lapse microscopy (e.g., stereomicroscope, confocal microscope, microCT) while keeping the samples intact. On select samples, cross-sections (e.g., billets and thin sections) of the samples are examined with microscopy (e.g., thin section, SEM, EDS) and bulk sample measurements (e.g., helium pycnometer, imbibition capacity) are acquired after reactive transport to quantify porosity changes with crystallization.

This presentation first details development of fabricated "lab-on-a-chip"miniature 3D synthetic rocks with varied reactive properties. The workflow enables control of porosity, permeability, microstructure, mineral composition, and accessible reactive surface area and allows for easier in-situ observations and measurements as opposed to real core experiments. Next, the presentation provides early insights on how formation of carbonates and carbonate mineralization proxies alters the microstructure of a rock and how to optimize injection strategies to maximize crystallization reaction and minimize permeability reduction. Results suggest that precipitation favors diffusion-dominated zones and that nucleation behavior and location will be influenced by liquid/gas interfaces and the presence of thin films. Results are cast in terms of dimensionless transport numbers (e.g., Capillary, Damkohler, Peclet numbers) and provide ideal benchmarks for numerical modeling and functional relationships for accelerating or inhibiting carbon mineralization within a porous media. Going forward, the 3D microfluidics setups will enable investigation of a host of coupled pore-scale alteration phenomena, including dissolution, carbonation/precipitation, and swelling/shrinking as a function of fluid flow/injection rates, pH, total dissolved solids, temperature, and pressure.

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MS13 / 792

Nanoporosity controls on the carbon storage and mineralization potential of basalts: insights from hydrothermal alteration at Newberry Volcano

Authors: Shaina Kelly[1]; Zuhao Kou[1]

Co-authors: Olivia Terry [1]; Tianxiao Shen [1]

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This study quantifies the pore structures and reactive flow capacity of basalt rocks, specifically a range of flow top (vesicular) and seal basalt samples from Newberry Volcano drill core (Oregon, USA). Dissolution and precipitation reactions in basalts and other mafic and ultramafic rocks (silicates rich in Mg, Ca, and Fe) are the foundation for carbon mineralization, in situ mining, and geologic hydrogen technologies due to high contents of reactive minerals (e.g., pyroxene and olivine) or critical minerals. However, despite their high reactivity, these rocks exhibit large variations in porosity and permeability. In fact, many of these rocks are nanoporous (<1um) or poorly connected, thereby challenging fluid access to critical and reactive mineral surfaces. The bulk volumes of qualifying basaltic and mafic/ultramafic rocks are vast, with the US's Pacific Northwest alone estimated to have 10^5 Gt CO2 basalt storage/mineralization capacity, assuming pore space and reactive minerals are accessible to fluid flow. Towards addressing accessible pore space and reactive minerals surfaces, this work examines the (a) pore size distribution and connectivity and (b) accessible mineral surface area within Newberry volcano basalt samples.

The Newberry Volcano basalts provide a natural laboratory for understanding multiphase and reactive flow potential of basalt pore structures. We collected 20 basaltic sandstone/volcaniclastic rocks and basalt/basaltic andesite rocks from USGS Newberry volcano drill core. The studied samples have been subjected to varied amounts of gases (CO2, H2S) and aqueous fluids in situ. The samples display varied degrees of hydrothermal alteration, where rock properties (porosity, permeability, lithology), temperature, and fluid composition dictate the extent of alteration. We characterize the macropores (vesicles) and nanopores (clays and matrix) of samples with N2 adsorption-desorption isotherms (BET surface area), TD-NMR T2, pycnometry, thin section and SEM/EDS, and microCT. The amount of Fe2O3, MgO, and CaO ranges from 18% (volcanic siltstone)-25% (flow-top basalt), confirming the reactivity of these Newberry volcano rocks. Direct numerical pore-scale simulations are used to study fluid flow capacity in image- and process-based domains for characteristic sample pore-scale features. We find distinct differences in pore structures among lithologies: for example, the volcaniclastic siltstones are dominated by a bimodal distribution, fresh/seal samples are dominated by a unimodal distribution, and multimodal distribution is significant in all hydrothermal altered basalts. Combining these distributions with imaging and modeling supports that nanoporosity is a driver of reactive flow capacity in basalts: Primarily nanoporous samples with extremely low permeability remain relatively "fresh"(unaltered) over geologic time. In originally more porous samples, aqueous fluids have altered primary minerals (plagioclase) into clays, quartz polymorphs, and carbonates which fill the pore systems, resulting in a secondary nanoporosity system. All studied hydrothermal altered basalts have similar pore size distribution and mainly contain slit-shaped pores (per BET analysis); the signal is likely dominated by clays. Overall, the natural CO2-fluid-rock system of the Newberry Volcano can be leveraged to understand anthropogenic CO2 movement in basalts. The alteration-nanoporosity-flow capacity feedback loop summarized in this work has implications for basalt storage capacity and seal performance for the aforementioned energy transition applications, especially CO2 storage and mineralization.

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MS03 / **793**

Dynamics of two-phase flow in coal using X-ray micro-computed tomography imaging and positron emission tomography

Authors: Joan Esterle[1]; Peyman Mostaghimi[None]; Ryan Armstrong[None]; Wen Xi[2]; YU JING[None]

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The fluid dynamics of gas-brine flow within porous media play a crucial role in the recovery of hydrocarbon gas and the sequestration of CO2. Coal seams are targeted as a reservoir rock because of their strong adsorption properties. However, permeability is an issue as they consist of matrix and fracture components, present a complex flow channel system for competing fluids and gases. During production, the initial dewatering process reduces pressure and induces CH4 desorption from the matrix into fractures, accompanying brine flow towards production wells. CO2 injection further displaces CH4 and stores CO2 in the matrix due to competitive adsorption with CH4. Moreover, Coal seams are dynamic during gas depletion and successive injection as the matrix shrinks and then swells, altering the structure of the flow channels. This introduces additional complexity to the transportation behaviour of the fluids. This study introduces an innovative approach to investigate the dynamics of gas-water two-phase flow within fractured coal cores. The methodology involves an integration of unsteady-state two-phase fluid flow experiments, dynamic positron emission tomography (PET) imaging, and high-resolution X-ray micro-computed tomography (micro-CT) imaging. Under reservoir pressure conditions, micro-CT imaging is employed to capture the fracture structure of the coal sample. A gas-injection-based unsteady-state flooding test is subsequently conducted on a water-saturated sample at the same pressures, with PET scanning used for dynamic imaging of the displacement process. This flooding experiment is designed to emulate gas-water transport behaviour in a coal seam during production, facilitating real-time data collection of gas injection volume, inlet-outlet differential pressure variations, and water production. The obtained data is utilized to predict the relative permeability curves of the sample. Following the flooding experiment, a multiscale image analysis is performed by aligning low-resolution PET images at different time steps with the high-resolution micro-CT image. it superimposes the flow path onto the fracture structure of the sample, allowing for the determination of water saturation and characterization of flow behaviour. This analysis leverages the unique advantages of PET's dynamic imaging capabilities and micro-CT's high image resolution to enhance the visualization of fluid transportation behaviour within the media. Overall, this approach offers significant potential for sensitivity analysis on relative permeability of a porous media, including not only coal, but also reservoir rocks like sandstone and shale. It can consider factors such as stress, temperature, and wettability, enabling a quantitative comparison of relative permeability and offering visual insights into fluid flow behaviour as conditions change. This contributes to precise predictions of relative permeability, aiding in the identification of optimal scenarios for both hydrocarbon exploitation and carbon sequestration.

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Poster / **795**

Retention Mechanism of Residual Oil in Different Pore-Throat Structures Under High-Flux Water Displacement Using Pore-Scale Two-Phase Flow Simulation Considering Dynamic Contact Angle

Author: Gaofei Yan[1]

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Objectives/Scope（25-75words）
High-flux water displacement is one of the effective methods for low-cost development of mature oilfields. The wettability alteration under high-flux water displacement is the crucial reason for improving displacement efficiency, which makes complex flow characteristic in different pore-throat structures. The objective of this paper is to establish a high-flux water displacement pore-scale simulation method considering dynamic contact angle to determine the distribution pattern and retention mechanism of residual oil.

Methods/Procedures/Process (75-100words)
Firstly, the physical models of different pore-throat structures (200mD and 50mD) were constructed by the extraction of the casting thin-section images. Then, the pore-scale two-phase flow mathematic model coupling the Navier-Stokes equation and the Phase-Field equation was established to track the phase interface migration. Moreover, a dynamic contact angle equation was added to the model. Finally, the commercial software COMSOL is used to solve the model by finite element method (FEM). Especially, the injection rate set to 2.25×10-8m3/s, the simulation time of high-flux water displacement set to 800s (about 200PV), and the contact angle change rate set to π/1200 rad/s.

Results/Observations/Conclusions (100-200words)
The results show that the displacement efficiency after high-flux water displacement is significantly improved when considering the dynamic contact angle. For the high permeability reservoir (200mD) with large pores and better connectivity, the oil in small throats near the main streamlines started to be displaced when the contact angle drops to 4/9π. The cluster-type residual oil remain oil in the weak sweep area is partially driven out when the contact angle dropped to 1/3π. The residual oil saturation at 200PV is reduced by about 15% compared to that at 30PV (traditional water displacement experiment). There are three main streamlines parallel to the injection-production direction, and the residual oil is mostly cluster-type oil far from the main streamlines. For the low permeability reservoir (50mD) with narrower pores and poor connectivity, the residual oil saturation at 200PV is reduced by about 7% compared to that at 30PV. There is only one main streamline connecting the inlet and outlet, and the residual oil is widely distributed near the main streamline.

Novelty/Additive Information (25-75words)
In this paper, a pore-scale long-time simulation method was established by coupling a dynamic contact angle equation to characterize the retention mechanism of residual oil under wettability alteration during high-flux water displacement. The impacts of pore-throat structure and displacement flux on the distribution pattern of residual oil were analyzed, which could provide valuable insights for improving the oil recovery (IOR) of mature oilfields developed by water flooding.

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798

Reclaiming Pharmaceuticals: Innovations in Wastewater Treatment

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Emerging contaminants (ECs, or micropollutants) are a diverse group of compounds and substances with significant environmental implications due to their potential toxicity 1. This category encompasses various substances, including active pharmaceutical ingredients. These specific contaminants enter urban waterways primarily from diffuse sources (e.g. households) and point sources (e.g. manufacturing plants, hospitals, clinics). Addressing these specific sources rather than solely relying on wastewater treatment plants could vastly improve treatment efficiency, reduce remediation costs, and prevent the creation of harmful byproducts downstream –a concept often referred to as "Turning off the tap"[2, 3]. Adsorption systems, commonly utilized in water treatment and purification, offer a substantial advantage by effectively removing contaminants, thereby preventing the generation and discharge of harmful byproducts [4]. To this end, we investigated adsorption technology as a potential mean of achieving high treatment efficiencies, both in batch and column lab-scale configurations, using simple as well as complex aqueous matrices. We also investigated the potential for recovery of the adsorbed compounds from the spent sorbent material, achieving promising results for future reuse and recycle-based approaches to pharmaceutical pollution.

1 J. L. Wilkinson and e. al., "Pharmaceutical pollution of the world's rivers," Proceedings of the National Academy of Sciences, vol. 119, no. 8, 2022.
2 J. L. Kormos, M. Schulz, H.-P. E. Kohler and T. A. Ternes, "Biotransformation of Selected Iodinated X-ray Contrast Media and Characterization of Microbial Transformation Pathways," Environmental Science & Technology, vol. 44, pp. 4998-5007, 2010.
[3] A. Nowak, G. Pacek and A. Mrozik, "Transformation and ecotoxicological effects of iodinated X-ray contrast media," Reviews in Environmental Science and Bio/Technology, vol. 19, pp. 337-354, 2020.
[4] A. Sengar and A. Vijayanandan, "Comprehensive review on iodinated X-ray contrast media: Complete fate, occurrence, and formation of disinfection byproducts," vol. 769, no. 144846, 2021.

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Poster / 800

The displacement of immiscible two-phase fluids in a pore doublet system

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Multiphase fluid flow in a pore doublet is a fundamental problem and is important for understanding the transport mechanisms of multiphase flows in porous media. During the displacement of immiscible two-phase fluids in a pore doublet, the transport process is influenced not only by the capillary and viscous forces, but also the channel geometry. In this work, a mathematical model and numerical simulations are presented for the two-phase fluid displacement in a pore doublet with considering the effects of capillary force, viscous force, and the geometric structure. These lead to new and more general analytical and numerical solutions for the pore doublet system, and it is found that the displacement process is dominated by the capillary number, viscosity, and radius ratios. The results can be used to explain and understand the preferential flows in porous media, such as for improving oil recovery from porous media; these are usually observed in oil recovery, groundwater pollution, and the geological sequestration of carbon dioxide.

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A Pore-Scale Simulation Study of CO2 Sequestration in Saline Aquifers using the Lattice Boltzmann Method

Authors: Hongwei Niu[None]; Yunfan Liu[1]; Zihan Hou[None]; lei li[1]; yongmao hao[None]; yuliang Su[1]

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CO2 geological storage, a prominent technology for mitigating greenhouse gas emissions, is often accompanied by significant capillary trapping phenomena in saline aquifers, thereby influencing reservoir utilization efficiency. In this study, the lattice Boltzmann method (LBM) based on the single-relaxation-time model (LBGK) is employed, utilizing the pseudopotential (Shan-Chen) multi-component model to simulate two-phase water-gas flow. Laplace's law is employed to determine the appropriate water-gas interfacial tension and the corresponding G values. The research investigates the migration process of CO2 and reservoir fluids in saline aquifers, analyzing the impact of capillary trapping on the CO2 storage capacity. The simulation explores various factors including injection direction, fluid viscosity, injection velocity, and wall wetting properties.Results indicate that as the fluid viscosity ratio increases from 5 to 10, the breakthrough time for CO2 decreases by 21.56%. With an increase in the injection velocity of CO2 from lattice speed 0.1 to 0.3, capillary trapping of CO2 significantly intensifies, resulting in a 34.09% reduction in CO2 spreading coefficient. As wall wetting properties transition towards CO2, the contact angle continuously decreases, indicating a weakening trend in CO2 capillary trapping. Within the contact angle range of 130° to 60°, the spreading coefficient of CO2 increases by 15.73%. Compared to injection parallel to the dominant channels, simulating injection perpendicular to the dominant channels results in a permeability that is 43.61% of the parallel case. The decrease in permeability helps suppress CO2 capillary trapping, with simulation results showing a 27.61% reduction in the distance between the leading and trailing edges of the water-gas interface when injecting perpendicular to the dominant channels.The study concludes that low injection rates, lower water-gas viscosity ratios, lower permeabilities, and surfaces favoring CO2 wetting are more suitable for CO2 storage in saline aquifers.

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Experimental investigation of CO2 diffusion characteristics in fractured volcanic cores

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Countries around the world have increased the exploration and development efforts for unconventional oil and gas resources, among which volcanic reservoirs as a considerable oil and gas resource have gradually been taken seriously. Compared with conventional reservoirs, fractured volcanic reservoirs have complex physical properties and developed natural fractures, making their development more difficult. The main exploitation methods include water flooding, gas flooding, gas injection and cyclic steam stimulation. CO2 injection has been proven to be an effective method for developing volcanic reservoirs. Its exploitation mechanism mainly includes diffusion, reducing crude oil viscosity, extracting light hydrocarbons, and reducing interfacial tension. Therefore, investigating the diffusion characteristics of CO2 in fractured volcanic reservoirs is of great significance for clarifying its exploitation effect and mechanism. In this paper, a high-temperature and high-pressure diffusion experiment device designed independently was used to conduct diffusion experiments of CO2 in saturated oil-bearing cores. A mathematical model for the diffusion of CO2 in saturated oil-bearing cores was established, and the diffusion coefficient of CO2 was calculated based on experimental data. The diffusion law of CO2 under different pore characteristics was analyzed. The results showed that the diffusion of CO2 in saturated oil-bearing cores experienced rapid diffusion stage, slow diffusion stage, and eventually reached equilibrium stage. The permeability and pore characteristics of the rock had a significant impact on the diffusion of CO2. Fracture could effectively connect isolated pores within the core. Under conditions with fractures, the diffusion coefficient was in the order of 10-9 m2/s, while the diffusion coefficient of cores without fractures was 10-10 m2/s. The size of the diffusion coefficient was positively correlated with permeability. In addition, pressure and diffusion radius also had a certain influence on the diffusion of CO2.

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Experimental invetigation on bioenzyme enhanced plugging removal and oil recovery in low permeability reservoirs

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Aiming at the problems of low permeability reservoirs, such as ‘injection failure and production failure’, incomplete fracture fluid backflow and rubber breaking, and reservoir plugging, the integrated technology of plugging removal and oil recovery with bioenzyme system is proposed. Compared with traditional fracturing fluid breaking agents and conventional water flooding, biological

enzymes have the advantages of high efficiency, green cleaning and so on, and have good application potential in low permeability reservoirs. Based on the viscosity degradation experiment of crude oil and guar gum fracturing fluid, two kinds of bioenzymes were screened for compounding, and subsequent core plugging and oil displacement experiments were carried out with the combined biological enzymes. Core permeability before and after plugging was measured by the core plugging test to evaluate the plugging effect of the combined enzymes, and the oil displacement effect of the biological enzyme system was evaluated by calculating the recovery rate. The experimental results show that 0.8g/L biological enzyme (amylase: mannanase = 1:1, mass ratio) has a good plugging and oil displacement ability. Under the condition of 50℃, after the combination of enzyme plugging, the core permeability can recover to a certain extent, and the displacement pressure is reduced. In terms of oil displacement, the experiment shows that the combination of enzyme can improve the oil recovery. The results of laboratory study on the compound bioenzyme system can provide a theoretical basis for the field application of bioenzyme plugging removal and oil recovery integration technology.

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MS08 / **808**

Experimental and Numerical Study of Carbon Dioxide Geological Storage in Coal –A Comparative Analysis with the application of Positron Emission Tomography Imaging.

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Co-authors: Kunning Tang [2]; Peyman Mostaghimi ; Ryan Armstrong ; Ying Da Wang [2]; YU JING

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With the global energy mix predominantly fossil fuel based¹, carbon dioxide (CO₂) capture, utilisation and geological storage (CCUS) is a key tool in reducing anthropogenic CO₂ emissions. One of the main challenges facing CCUS in coal seams is the loss of injectivity due to CO₂ coal swelling^{2–7}. This work aims to improve the understanding of CO₂ transport mechanisms in coal by applying in-situ Positron Emission Tomography (PET) imaging to obtain direct images of CO₂ flow in coal, allowing for better CO₂ geosequestration techniques.

This work presents a comparative history matching analysis between a one-dimensional Advection Diffusion Equation (ADE) model and experimental data obtained from in-situ PET imaging during core flooding. Traditional core flooding methods usually rely on assumptions that flow within samples is piston like, possibly leading to inaccuracies during modelling⁸. The use of PET imaging provides an actual representation of gas flow behaviour and serves as a ground truth point of reference during history matching. This comparative analysis focuses on determining how the diffusion coefficient of CO₂ in coal changes vis-à-vis coal properties such as initial adsorbate molecules, coal swelling and their effects on gas (particularly CO₂) diffusion within coal samples.

[¹¹C]CO₂ was utilised as the PET radiotracer during core flooding experiments to directly image carbon dioxide (CO₂) diffusion dynamics and mechanisms within coal samples. A 1-D ADE model in MATLAB was then history matched to experimental data for the purpose of obtaining the diffusion coefficient that best represented what was observed. Additionally, X-Ray μCT imaging technology was utilised to obtain high resolution (30μm) images of the core samples. Machine learning algorithms were then applied to these CT images as a method of digital image segmentation to obtain a good estimate of sample porosity, further improving the accuracy of the 1-D ADE model. In-situ PET scans allow for a dynamic observation of gas flow during the core flooding experiment as well as a source on which gas diffusion effects can be confirmed through the use of history matching with a 1-D ADE model in MATLAB and subsequently back calculating the diffusion coefficient of best fit from the ADE model that accounts for key core flooding parameters such as coal porosity, gas flow rate and type of injected gas.

The results show that stable diffusion coefficients arise when samples are dry and an inert gas (He) is used as the carrier gas. In the cases of competitive adsorption between methane (CH₄) and CO₂ in samples that were CH₄ saturated show a decreasing diffusion coefficient. Diffusion coefficients in CO₂ saturated samples were in the order of 100 times lower than in samples that were not exposed to CO₂ prior to injection. This indicates that coal swelling has a significant impact on the ability of gas to effectively diffuse in the coal matrix. These findings further develop the body of knowledge surrounding CO₂ geosequestration in unmineable coal seams and contributes to the optimisation of CCUS processes during the transition to low-carbon and renewable energy sources.

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Effect of shale pore structure on oil and CO_2 two-phase flow based on FIB-SEM and PNM

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CO_2 injection development in shale oil reservoirs, employed for enhancing shale oil recovery and sequestering CO_2 underground, represents a promising synergy of bolstering oil extraction and environmental preservation. With the development of nanoscale core scanning technology, the oil-CO_2 fluid movement characterization in CO_2 displacement under real shale porous media has needed to be re-cleared. In this research, based on the pore network modeling (PNM), with different pore structure network extractions in shale of different lithologies. We quantified the pore structure characteristics and elucidated the effect of the oil and CO_2 flow capacities, and further specified the mechanism of CO_2 movement to the oil phase.

Firstly, the digital cores of quartz-rich shale, carbonate-rich shale, and high clay content shale were established using FIB-SEM scanning technology and extracted pore networks to analyze pore spatial characteristics such as porosity, tortuosity, pore-throat ratio, and coordination number, with different lithologies. And further quantified using a generalized extreme value distribution. Secondly, a modified Young's equation at the nano-scale was used for capillary pressure correction, which in turn led to the construction of a pore network model applicable to nano-scale oil-CO_2 flow. Finally, the microsimulation of oil and CO_2 flow within the three-dimensional shale porous medium was carried out, the oil and CO_2 relative permeability and phase flow rate under different pore structures was calculated, and the fluid mobilization mechanism of shale pores was analyzed, which led to the evaluation of the development effect.

According to the results of the study, quartz-rich shale has the highest coordination number, the largest porosity, and the best connectivity compared to carbonate-rich shale and high-clay content shale. Among them, porosity and coordination number are positively proportional to the recovery rate, while tortuosity and pore-throat ratio are inversely proportional to the recovery rate. The variation of oil and CO_2 flow capacity is more pronounced in nanopore sizes (especially less than 50 nm) than in micrometer pores. Compared with conventional aqueous media, CO_2 is more effective in mobilizing crude oil within small pores, increasing oil phase permeability and further enhancing crude oil recovery with an average recovery of up to 90.1 %.

In this paper, the spatial distribution characteristics and mobilization mechanism of oil and CO_2 under different shale pore structures are analyzed by the pore network modelling for the nanoscale, which helps to understand the two-phase flow law of oil and CO_2 in shale reservoirs from the microscopic scale.

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MS06-B / 814

Interface Evolution During Pore Water Evaporation in Micromodels

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The interface between liquid and vapor phases within porous media plays a pivotal role in enhanced vapor diffusion and water evaporation. The liquid-vapor interfaces can be classified into internal interfaces (pertaining to vapor diffusion) and external interfaces (associated with phase change) based on their distinct mechanisms. However, the intricate geometric and topological complexities within these interfaces pose challenges in discerning between their internal and external manifestations, hindering a comprehensive understanding of heat and mass transfer mechanisms within soil pores. In this study, a meticulously engineered Hele-Shaw cell integrated with patterned micropillars offers an innovative approach for comparing interface evolution in pores with diverse patterns. A sophisticated image-processing analysis was employed to accurately compute the evaporation rate of the pore water from the micromodels. Equivalent lengths were obtained to determine interface areas at distinct time intervals. Comparison of the continuous recession of the liquid-vapor interface in a stable micropillar pattern to the air-entry of the internal interface and pinned external interface in an unstable micropillar pattern provides an approach to quantitatively separate the internal and external interfacial evaporation rates. Furthermore, employing image processing during evaporation enables the calculation of both global and local interface curvatures. Consequently, a correlation between the characteristic curvature radius and the averaged interfacial evaporation rate was established, consistent with prior experimental findings documented in the literature. The distinction between internal and external evaporation rates offers a fresh perspective, shedding light on the mechanisms that drive enhanced evaporation and diffusion within porous media.

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Poster / 815

Numerical study of the gas-liquid separation of cryogenic fluids with porous structures

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Abstract
Gas-liquid phase separation based on the porous media is vital for the stable operation of rocket engines in microgravity. To reveal the mechanism of nonisothermal phase separation with the porous media, a pore-scale numerical simulation is conducted to investigate the gas breakthrough at the porous array structure. Liquid oxygen and oxygen vapor are taken as the working fluids. The phase-field method is adopted to capture the gas-liquid interface. The influences of the inlet temperature and solid-liquid heat transfer on the flow characteristics are investigated. The results show that the bubble size increases rapidly under superheated inlet temperature when compared to that under subcooled inlet temperature. Without considering heat transfer, the critical pressure increases with the increase of the inlet temperature. Under subcooled inlet temperature, the condensation rate is reduced with the increase of the heat flux, and even the evaporation rate is stronger than the condensation rate. The bubble breaks into small daughter bubbles easily under high heat leakage due to the increasing size. The transit time is dependent on the bubble behavior, which is related to the driving pressure, inlet temperature, and heat leakage. The synergetic effect of inlet temperature and heat flux on the critical pressure shows that the critical pressure is more dependent on the inlet temperature when compared with the heat leakage.

Keywords: cryogenic propellants, phase change, porous structure, critical pressure, phase-field method

Acknowledgements
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Multiscale Simulation Study on Residual Trapping in Subsurface Rocks with Clay Minerals: Implications for Geological Carbon Storage

Authors: Sheng Li[1]; Yunfeng Liang[2]; Fei Jiang[3]; Takeshi Tsuji[2]; Haihu Liu[1]; Keishi Usui[4]; Tomohiro Taniguchi[4]; Gyuhwan Jo[4]

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Geological carbon storage is a promising and feasible technique for greenhouse gas mitigation. To improve CO2 storage efficiency and develop monitoring techniques, it is important to know the CO2 flow behavior and capillary trapping mechanisms in subsurface rocks. Clay minerals, often found in sandstone, may exert a vital impact on the displacement process. However, the diversity of rock components, notably clay minerals, has been consistently overlooked in previous studies. In this study, we presented a new concept, namely, digital rock physical chemistry, by integrating molecular-scale and pore-scale simulations to investigate CO2 residual trapping mechanisms in porous systems, for high-efficiency geological carbon storage. A digital rock with kaolinite clay minerals is used for the porous media. The decane, CO2, and their mixtures are used as the fluid to be displaced. The intrinsic physicochemical properties, including the fluid viscosity, the fluid-water interfacial tension, and the fluid-water-mineral wettability at varying CO2 concentrations, are investigated using molecular dynamics simulation. These molecular-scale properties are then upscaled into a core/pore-scale system with the help of lattice Boltzmann simulation. The results are summarized into a 3D phase diagram, which reveals the non-monotonic variations of the initial-residual (I-R) curves across different CO2 concentrations. Although the obtained I-R curves in oil and CO2 displacement exhibit similar trends, the trapping characteristics, including residual saturation and fluid distributions, differ. These findings underscore the critical roles of molecular scale interfacial phenomena and rock surfaces, particularly those related to kaolinite clay minerals, in subsurface multiphase seepage and geological carbon storage, highlighting the importance of digital rock physical chemistry.

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MS03 / 820

Effect of non-acid-soluble minerals on acid-etched hydraulic fracture morphology and conductivity for acid-fracturing in carbonate rock

Authors: Bo Gou[1]; Zihao Liu[1]; Jianchun Guo[1]; Bin Xiao[1]; Kun Pu[1]

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Acid fracturing is a primary stimulation technique for carbonate reservoirs. Acid selectively etches hydraulic fractures, forming high-conductivity channels capable of transporting oil and gas under the influence of normal closure pressures. Numerous fracture acidization models have focused on factors such as reservoir temperature, acid fluid type, and distribution of carbonate minerals, but few have explored the impact of non-acid-soluble minerals, such as talc and quartz, on the fluid-flow and reaction mass-transfer mechanisms within hydraulic fractures in carbonate reservoirs.
This study developed a hydraulic fracture acidization model that considers the influence of non-acid-soluble minerals, and the model was validated through laboratory-scale API rock plate acidization experiments. Furthermore, the study extensively discussed and analyzed the effects of non-acid-soluble minerals on acid etching of fractures.
The results demonstrate that the model effectively captures the acid etching characteristics of hydraulic fracture walls containing non-acid-soluble minerals. Non-reactive minerals on the hydraulic fracture walls influence the flow paths of the acid and the diffusion rate of hydrogen ion, leading to non-uniform dissolution on the fracture surfaces and the formation of rough fracture faces. Non-acid-soluble minerals retards the rate of acid-rock reaction, and as their content increases, the extent of surface dissolution on the fractures gradually diminishes, resulting in a reduction in non-uniform etching. However, non-acid-soluble minerals can act as a support for the fractures after closure, to some extent enhancing both fracture conductivity and its sustaining capacity.
This study reveals the impact of non-acid-soluble minerals on the acid etching morphology and conductivity of hydraulic fracture, providing valuable insights for the design of acidizing process design in carbonate reservoir.

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821

Quantitative characterization on pore structure evolution and mechanical properties during in-situ conversion of medium-low maturity shale

Authors: Yaqian Liu[1]; Chuanjin Yao[1]; Qi Zhang[1]; Yangyang Xuan[1]; Jiao Ge[1]

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In-situ conversion technology has emerged as a pivotal method for the exploitation of medium-low maturity shale reservoirs. Upon thermal stimulation of the shale reservoir, there is a notable conversion of unconverted kerogen and undischarged heavy hydrocarbons into valuable pyrolysis oil and gas. This is a thermal-fluid-solid multi-field coupling process, accompanied by the expansion of existing fractures and the generation of new ones, resulting in changes in the pore structure and mechanical properties of medium-low maturity shale, which significantly affect the seepage of thermal fluids and the release of pyrolysis oil and gas. In this paper, in-situ conversion experiments under different pyrolysis final temperatures were conducted on medium-low maturity shale core samples from the Chang 73 section of the Ordos Basin. The pore structure of shale before and after in-situ conversion was determined by nuclear magnetic resonance means and the permeability was calculated. Multiple testing methods were further employed to quantitatively characterize various mechanical properties. A quantitative characterization model of pore structure evolution and mechanical properties during the in-situ conversion of medium-low maturity shale was derived through nonlinear fitting. The results indicate that with the increase in the pyrolysis final temperature, pore space becomes larger, the porosity and permeability of the medium-low maturity shale exhibit varying degrees of enhancement, while the thermal conductivity, compressive strength, and tensile strength decrease. The variation in the rock elastic modulus can be characterized in segments. This study elucidates the response of the pore structure and mechanical properties of medium-low maturity shale to pyrolysis temperatures, providing a foundational model for the evolution of various properties in the multi-field coupled simulation of in-situ conversion.

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822

Study on the microscopic interaction mechanism between CO2-nanoparticle composite system and shale oil

Author: zhiwen yang[1]

Co-authors: lei li [1]; yuliang su [1]; dian zhang [1]; xue zhang [1]; zhaoxue huang [1]; xinhao wang [1]

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CO2 oil drive technology is one of the most promising methods to improve recovery in unconventional reservoirs, but it is difficult to achieve CO2 mixed-phase in most of the reservoir conditions, while nanoparticles can effectively improve CO2 oil drive and reduce mixed-phase pressure, so the

CO2-nanoparticle composite system composed of both has a broader development prospect. In this paper, we propose to study the mechanism of CO2-nanoparticle composite system for oil repelling in unconventional reservoirs. Firstly, we analyze the effects of different types, particle sizes and concentrations of nanoparticles on rock wettability and oil-gas interfacial tension through wetting angle and interfacial tension experiments under high temperature and pressure. Secondly, the effect of SiO2 and ZnO nanoparticles on the effect of CO2 oil drive is investigated by micro-visualization experimental simulation technique to reveal the micro-action mechanism of the composite system to enhance the recovery of crude oil.
In this paper, microscopic experimental simulations of multiphase fluid repulsion experiments in real porous media of reservoirs are carried out on a two-dimensional glass etching model through a high-temperature and high-pressure microfluidic experimental platform to obtain the contact angle evolution on the pore walls, the parameters of interfacial tension of the formation and the interaction between fluids, and establish the parametric relationships of inter-fluid motion. The results show that nanoparticles can effectively act on the two-phase interface during microscopic repulsion in porous media, reducing the interfacial tension and improving the repulsion efficiency. Meanwhile, the diameter of nanoparticles and different nanoparticles have different effects on CO2 repulsion. In this paper, SiO2 and ZnO nanoparticles are used, and the reduction of nanoparticle diameter improves the repelling effect; in terms of reservoir properties, the larger the porosity, the better the sealing effect of nanoparticles, and the more obvious the effect of improving the recovery. By optimizing the nanoparticle concentration, diameter, gas injection method and injection rate, the recovery rate can be further improved by 5%-10%.

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MS03 / **823**

Dynamics of fluid flow in natural fracture networks

Authors: Cuong Bui[1]; Stephan Matthai[1]

[1] *University of Melbourne*

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In complex fracture networks, dynamic fluid-flow patterns arise already at flow velocities in the centimetre-per-second (cm/s) range. Yet, these phenomena get ignored or underestimated when such flows are modelled using Stokes'equation or steady-state approximations of the Navier Stokes equation (NSE) are used.
Here we apply the Detached-Eddy Simulation technique to solve the NSE in rock fractures, carrying out an investigation of the flow dynamics and flow micro-transitions in particular. Following verification and validation of this approximative model with data collected from physical flow experiments involving single Y- and X-shaped channel intersections, we have performed transient simulations on discrete fracture models constructed of tens-of-metre sized natural patterns with

millimeter-wide open fractures. Our new results obtained on highly refined two-dimensional fracture meshes with tens of cells spanning the width of each fracture reveal that fracture flow, that is typically represented by streamlines and pressure distribution patterns, becomes unsteady at cm/s velocities. Dynamic eddies emerge at various scales, occupying a substantial volume of the fracture channels, increasing the tortuosity of the flow and fluid distribution in fracture branches. Associated pressure fluctuations do not average out at the model scale but are detectable there, possibly reaching magnitudes of ~10% of the total pressure drop across the network. The contribution of inertial losses to the hydraulic head gradient across the network is substantially increased with the onset of non-stationary eddies, confirming that they are the primary source of flow nonlinearity.

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Poster / 824

Study on mechanism of removal of residual DNAPL by co-injection of ethanol and CO2 into 2D porous micromodel

Author: Min Yuan[1]

Co-author: Huirong Guo [1]

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Groundwater contaminated with dense non-aqueous phase liquids (DNAPLs) such as chlorinated hydrocarbons is difficult to remediate, and the effectiveness of conventional pump treatment techniques is very limited due to its low contaminant solubility. Enhanced in-situ flushing has attracted widespread attention as an alternative to the use of flushing fluid such as cosolvent and gas co-injection. It is very important to understand the recovery mechanism of cosolvent and gas co-injection into polluted aquifers to improve the recovery efficiency of polluted aquifers. In this study, the removal process of residual PCE in a two-dimensional (2D) micromodel that is used to represent the porous media with different concentrations of ethanol + CO2 and different flushing rates was observed by using a camera at room temperature and pressure, and the removal mechanism of DNAPLs under cosolvent + gas co-injection was preliminarily understood. Firstly, it was verified that increasing the concentration of ethanol solution could increase the dissolution rate of ethanol to PCE and promote the dissolution of residual PCE. Secondly, when the ethanol solution and CO2 were co-injected into the micromodel, the residual PCE in the injected CO2 flow channel migrated out of the micromodel, which also changed the distribution of PCE, but did not reduce the interface area between PCE and flushing solution in the pore channel. It is well known that the interfacial area is proportional to the dissolution rate, which means that the injected gas does not inhibit the dissolution of the ethanol to the PCE, so the remediation efficiency of the contaminated aquifer can be significantly improved. In addition, a small fraction of PCE remains in contaminated aquifers that are troubles to remove in the small pore channels or the dead end channels, and are hard to

completely repair with only cosolvent flushing. In the case of co-injection of ethanol solution with CO2, CO2 cannot enter these channels, but the ethanol solution can be sent into these channels to contact with PCE, promote the dissolution of PCE, and thus improve the removal rate of PCE in the aquifer. Finally, different experiments were compared, and it was found that when the injection flushing rate ratio of 60wt% ethanol to CO2 was 1:2, the removal rate of DNAPLs could be improved in a short time, and the amount of cosolvent could be saved, so as to obtain the best remediation scheme, which is of great significance for rapid repair and cost saving in the actual field.

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MS09 / 826

Pore-scale multiphase reactive transport and CO2 mineralization capacity in vesicular basalts

Authors: Shaina Kelly[1]; Tianxiao Shen[1]

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The geological storage of CO2 has emerged as a critical pathway for decarbonization, where in situ carbon mineralization in mafic/ultramafic rocks such as basalts is considered the most stable form of CO2 storage. in-situ CO2 mineralization pilot projects in basaltic formations include the Wallula project in Columbia River basalt and the Carbfix project in Icelandic basalt. Multiphase flow governs the invasion and distribution of native brine, carbonated water, and injected supercritical CO2 and will determine the accessibility and carbonation capacity of reactive mineral pore surfaces during geochemical processes. As such, what is the mix of injectate or injection scheme that optimizes tons of anthropogenic CO2 injected (storage) and mineralization capacity (security) for different formations?

We leverage pore-scale, multiphase computational fluid dynamics (CFD) models, enhanced by experimentally- and theoretically-informed reactive transport relationships and mineral-fluid wettability values, to assess the complex interplay between mineral hydrophilicity, capillary trapping, thin films, dissolution, precipitant nucleation, and mineralization. We simulate various injection schemes, including supercritical (dry) CO2 invading in-situ brine and water-alternating-gas (WAG) injection, within several representative vesicular basalt samples (including one fresh basalt sample, one from the Carbfix site, and two from different flow-top zones in the Wallula site). The pore-scale models are informed by petrographic data of pore morphology (e.g., thin section, SEM, micro-CT), physical-chemical mineralization behavior (coupled with PHREEQC), and routine core analysis data. The models are tuned with different boundary conditions and initial conditions to represent the basalt units in different locations in the reservoir under the selected injection schemes. For each sample, we quantify crucial

dynamic relationships for geologic storage and mineralization, including porosity-permeability, accessible reactive mineral surface area, brine-CO2 capillary pressure-saturation (Pc-Sw), and relative permeability (Kr-Sw) relationships. These relationships are explored as a function of native basalt groundwater composition, mineral-specific surface area, and the sequence of pore-scale alteration processes.
The aforementioned dynamic pore-scale relationships are integrated with fluid characterization and core-scale measurements, including hydraulic tests, helium pyconometry, and NMR measurements. Results indicate a strong correlation between the location of precipitated nodules and the menisci of CO2 bubbles under steady state, depicting a vital role of multiphase flow in understanding geochemical processes.
Ongoing efforts involve extrapolating pore-scale functional relationships to gridblock-scale reactive transport reservoir models (e.g., STOMP and MRST) to refine predictions of invasion depth, carbon storage and mineralization capacity, with the consideration of evolving accessible reactive surface area on a larger scale.

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MS20 / 830

Geometry of the porcine myocardial microcirculation with and without cardiac microvascular obstruction: preliminary results from an ex vivo study with propagation-based phase contrast tomographic microscopy

Author: Ross Straughan[1]

Co-authors: Eric Schreiber [1]; Anne Bonnin [2]; Nikola Cesarovic [1]; Dominik Obrist [3]

[1] *ETH Zurich*

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In cardiac microvascular obstruction (MVO), vessels of the myocardial microcirculation are fully or partially occluded such that the affected tissue is under-perfused. MVO may result from a catheter-based removal of a larger thrombus in a coronary artery after a heart attack. During the intervention, this thrombus may be broken up into small microthrombi, which are washed downstream with the re-established blood flow potentially occluding vessels of 200µm diameter or less.
Blood perfusion of the myocardium with MVO is governed by the geometry of the myocardial microcirculation. Both the distribution of vascular branchings at different vessel diameters and the network topology determine the location of the occluding microthrombi and their effect on blocking

the perfusion downstream of the occlusion. For example, the presence of collateral vessels (vascular loops) at the level of arterioles may allow the blood to bypass a local obstruction, whereas an occlusive microthrombus in a tree-like topology will block blood flow in the whole downstream region. Unfortunately, there is only limited knowledge on the geometry of the myocardial microcirculation. Microfluidic models rely on older histological data [1,2]. Moreover, there is even less knowledge about the distribution of microthrombi in MVO and whether they are fully occlusive or only semi-occlusive.
Therefore, we performed an imaging study using propagation-based phase contrast tomographic microscopy at the TOMCAT beamline of the Swiss Light Source (PSI, Würenlingen, Switzerland) on seven samples of pig hearts with and without MVO. These samples were obtained from a large animal trial with a porcine MVO model using microthrombi that were created by dissecting autologous arterial thrombi into small fragments of 150-300µm [3].
The imaging data with an isotropic voxel size of 1.625µm is segmented using the nnUnet [4] algorithm, which was trained with manually labeled data. Preliminary results indicate a complex vascular network with larger arteriolar vessels on the outer side of the myocardial wall (epicardium) that are branching into ever smaller vessels toward the inner side (endocardium). Furthermore, we could identify local microthrombi in arterioles of 50µm diameter. It is the aim to use fully automated segmentation to improve existing microfluidic models of MVO 2 which can help to develop novel treatment strategies for MVO.

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Poster / 831

Gas mass transfer in deep coal cleats: coupling multiple flow mechanisms and poromechanics with creep

Author: Tao Zhang[1]

Co-authors: Jianchun Guo [1]; Jie Zeng [1]; Zhihong Zhao [1]

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Deep coal rocks normally have higher gas content compared with shallow to medium-depth coal formations, showing great exploitation potential. However, they generally have complex pore structure and exhibits poor gas transport capacity under high overburden stress. The utilization of massive hydraulic fracturing can effectively release the productivity of deep coal reservoir. Nevertheless, the high overburden stress enhances the rock elasticity. Thus, during fracturing fluid flowback and the later long gas production periods, coal permeability loss due to matrix creep deformation in addition to the effective-stress-induced permeability reduction. Accurate characterization of deep coal rock permeability is an indispensable step toward precise simulation of gas transport and accurate assessment of productivity.

Coal permeability is mainly offered by the cleat system. To fully consider the impact of multiple gas transport mechanisms and creep on coal permeability evolution, this research presents a unified apparent permeability model based on the poromechanical theory and flow regime correction. Multiple flow mechanisms, including viscous flow, Knudsen diffusion, desorption, and real-gas effects are coupled in the single-fracture/cleat flux equation with dynamic viscosity. The fractal theory is employed for permeability upscaling. Specifically, the dynamic fracture/cleat aperture incorporates the impacts of desorption-induced internal swelling, full-stage/two-stage creep-induced compression and fracture/cleat aperture shrinkage depending on the actual stress state.

The proposed permeability model's results show good agreement with experimental data and can explain the time-dependent permeability evolution during the full-stage creep process. A new permeability surface concept is established to better illustrate permeability evolution by including the time dimension. During gas extraction, initially, permeability mainly influenced by the decelerated creep with the permeability drop gradually slows down. Then, rock creep deformation enters the steady stage, leading to a slight permeability change. The third-stage permeability evolution is caused by the accelerated creep that only appears when the effective stress is excessed the yield stress. To clarify the competitive effects of multiple gas transport and rock deformation mechanisms on deep coal cleat permeability, a novel controlling mechanism diagram was proposed with three realms for the creep-dominated region, gas-pressure-dominated region, and the desorption-dominated region, respectively. The contributions of different gas transport mechanisms on permeability evolution during different pressure and time scales were further analyzed. Due to the analytical feature, this model can be easily inserted into fully-coupled numerical simulator to predict deep coal rock gas production.

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MS08 / 832

Cotransport of clay and microplastics in saturated porous media

Author: Mahima Horta[1]

Co-author: Seetha N [1]

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The widespread use of plastics for various applications lead to their inevitable release into the environment. The disintegrated microplastics particles may ultimately find their way into the subsurface, thereby contaminating soil and groundwater. Hence, it is essential to understand the transport behaviour of microplastics in soil to protect drinking water wells from contamination. The presence of natural colloids such as clays in the subsurface are known to alter the transport behaviour of several contaminants. This study aims to understand the cotransport of clays and microplastics in saturated soil through column experiments and mathematical modeling. Experimental results showed enhanced transport of microplastics and retarded transport of clays during their cotransport as compared to their individual transport. This contrasting transport behaviour of clays and microplastics during their cotransport may be due to the competition between them in finding deposition sites on grain surfaces and also due to the formation of clay-microplastics heteroaggregates which may have different surface properties than individual clay and microplastics particles. The experimental results were successfully simulated using mathematical model which accounted for clay and microplastics retention in soil, heteroaggregation kinetics, and heteroaggregate retention in soil.

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MS01 / **833**

Investigation of the effect of capillary number, working pressure and hysteresis on hydrogen storage and recovery efficiency using a CFD approach

Authors: Matin Bagheri[1]; Hassan Mahani[1]; Shahab Ayatollahi[1]

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A crucial aspect of maximizing hydrogen storage and recovery in aquifers is understanding the flow dynamics of hydrogen-water. By gaining insights into these interactions at the pore scale, researchers can develop more efficient strategies for optimizing storage capacity and extending the production life span in aquifers. This progress ultimately contributes to advancing underground hydrogen storage technologies for practical applications. This study uses computational fluid dynamics (CFD) simulation to investigate the impact of flow regime, pressure, compressibility, and hysteresis on the pore-scale flow patterns of hydrogen-water and recovery efficiency during underground hydrogen storage. The findings indicate the hydrogen-water displacement efficiency is significantly affected by the capillary number. We found that different flow rates are favorable during hydrogen injection and production, and that a medium flow rate corresponding to specific capillary numbers can minimize capillary and viscous fingering mechanisms, leading to improved storability and recovery factor. It was shown that the expansion of gas near the outlet of the porous medium alters the local flow patterns, specifically at low-pressure systems. This highlights that during low-pressure experiments, this effect may go unnoticed and that can potentially impact the storage and withdrawal efficiency of hydrogen. Additionally, the research reveals that trapped hydrogen bubbles can create a “self-cushion effect” during the cyclic process, which is eliminated at capillary numbers higher than 10^(-4). While no consistent trend was observed for the effects of this phenomenon on the hydrogen recovery factor, the results indicate a slight enhancement of hydrogen storability in the 3rd cycle due to the self-cushion effect.

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Poster / 834

Coupled studies of oil compositions and storage spaces in the Kongdian Shale Formation, Bohai Bay Basin, Eastern China

Author: Weixing Yan[1]

Co-authors: Qiming Wang [1]; Qinhong Hu [1]; Shengyu Yang [1]; Xuyang Wang [1]

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The shale in the Kongdian Formation, Bohai Bay Basin is one of the leading shale oil targets in China and attracted attention from both industry and academics since the 2010s. Shale oil is known to distribute in the μm to nm pores in the shale formations. The oil compositions and pore spaces of shale formations strongly influence the shale oil production behavior for an efficient development. The four components of shale oil (saturates, aromatics, resins, and asphaltene) and pore space of shale have been studied separately in many previous researches. However, the combined distribution of different shale oil compositions in the pore spaces has rarely been studied. To investigate the

storage space of different compositions of shale oil, t, this study combined organic geochemical and petrophysical methods for core samples of Kongdian Formation. Extracts were collected after the 1st, 5th, 10th, and 30th day of solvent extraction, then analyzed by bitumen extraction and separation and GC-FID to determine the composition changes vs. time. Shales were collected at the same time interval to investigate the pore structure changes vs. time by mercury intrusion porosimetry and nitrogen adsorption. Results show that as the solvent extraction time gets longer, (1) the main composition of extracts changes from saturates to resins, and saturates gradually become heavier, (2) the porosity of shale gradually increases, and pore space first mainly increases in the μm-nm pore, then mainly increase in nm pores. In summary, this study is important to understand the distribution of different shale oil compositions and provide fundamentally important knowledge in reservoir evaluation.

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MS13 / **836**

Fractal nanopore structure of anthracite and CO2 adsorption-induced alteration: A synchrotron radiation SAXS study

Author: Yixin Zhao[1]

Co-author: Xiaodong Guo [1]

[1] *China University of Mining and Technology (Beijing)*

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Abstract:
Coal is a porous medium material with a highly developed pore network inside. Nanopores dominate gas adsorption and transport behavior in geological reservoirs. The fractal nanopore structure of anthracite from the Qinshui Basin were characterized using synchrotron radiation small angle X-ray scattering (SAXS). Based on the fractal theory of SAXS, the fractal characteristics of nanopores were obtained by analyzing the scattering data. The results indicate that the nanopores at 10~70 nm exhibit surface fractal characteristics, with irregular self-similar surfaces. The fractal nanopore structure of different sizes can be obtained by dividing the logarithmic curve into different regions. The pores at 10~20 nm, 20~30 nm, and 30~40 nm exhibit surface fractal characteristics, with the greatest contribution to the surface fractal characteristics of the overall pores (10~70 nm). However, the pores at 40~50 nm, 50~60 nm, and 60~70 nm exhibit pore fractal characteristics, reflecting the self-similar pore structure of the nanopores. Compared to the initial state, the surface fractal dimension of pores at 10~70 nm with CO2 adsorption gradually decreases. There is a negative correlation between surface fractal characteristics and adsorption pressure. From the initial state to 3 MPa adsorption, the fractal dimensions of pores at 10~20 nm, 30~40 nm, and 60~70 nm decreased by 5.597%, 2.397%, and

8.214%, respectively. CO2 adsorption weakens the fractal characteristics most significantly. The fractal dimensions of pores at 20~30 nm and 50~60 nm exhibit fluctuations under different adsorption pressures. CO2 adsorption has a relatively small impact on the fractal nanopore structure. Specifically, the pores at 40~50 nm with CO2 adsorption have the maximum fractal dimension (up to 2.97) and remain constant. It is difficult to alter the self-similarity of pore structure between 40~50 nm for CO2 adsorption.
Key words: Coal; Nanopore; CO2 adsorption; SAXS; Fractal

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Poster / 837

Numerical simulation on the four-dimensional in-situ stress evolution in shale gas reservoirs under water injection

Authors: Qi Ruan[1]; huiying tang[1]; shangui luo[1]; yulong zhao[1]; zehao xie[1]

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The rapid decline in production from shale gas wells necessitates the implementation of infill drilling and refracturing technologies to effectively utilize the remaining reserves. These techniques are crucial for maintaining long-term stability and increasing production in gas fields. As reservoir depletion occurs and water injection is implemented, geo-mechanical parameters such as reservoir pressure and in-situ stress undergo changes. These changes lead to distinct fracture propagation behaviors between old wells and those that are newly infilled or refractured, significantly impacting the strategies for future infill well deployment and refracturing operations. To predict the geometry of fractures in refractured and infilled wells with precision, an in-situ stress evolution model for the entire cycle from hydraulic fracturing to reservoir depletion in shale gas horizontal wells was established. This model utilizes water injection methods to simulate the injection of fracturing fluid and adjusts the stress-sensitive curves of fractures and matrix to match the fracturing operation pressure. It also reconstructs the pore pressure and saturation distribution field post-fracturing, facilitating further dynamic simulation of post-fracturing production and enabling a comprehensive depiction of the impact of in-situ stress throughout the entire fracturing and production process.
Research results indicate that the injection of fracturing fluid significantly affects the pressure and stress variations both inside and outside the fractures, with different patterns of stress changes. The differential horizontal stress increases inside the fracture, with the maximum increase occurring at the fracture tips, and decreases along the sides of the fracture, returning to the initial value as the distance from the fracture increases. If the injection of fracturing fluid is not considered, the differential horizontal stress decreases both inside and on the sides of the fracture, with a slight increase at the fracture tips. Under both scenarios, the stress changes during reservoir depletion also differ: overall,

the principal horizontal stress decreases, with the minimum horizontal stress differential occurring inside the fracture. Moving towards the sides, the horizontal stress differential gradually increases and then decreases, approaching the initial value. When considering the injection of fracturing fluid, the changes in stress magnitude are relatively smaller, and the deflection angle of stress direction is correspondingly smaller. Pre-fracture water injection can significantly restore the pressure and stress state of the depleted zone, but an increase in injection volume does not necessarily enhance the fracturing modification effect. Optimizing the injection volume and the well soaking time before fracturing are key to improving fracturing efficiency.
By utilizing a four-dimensional in-situ stress evolution numerical simulation method that takes into account the entire cycle of fracturing production in shale reservoir horizontal wells, it is possible to elucidates the effects of initial fracturing, subsequent production, and water injection on reservoir in-situ stress. It offers crucial guidance for the design of refracturing in horizontal shale gas wells and strategic infill well placement.

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Investigation on influence of supercritical water treatment on pore structure characteristics of Chang 73 medium-low maturity shale

Authors: Fanyi Meng[1]; Chuanjin Yao[2]; Baishuo Liu[2]; 娇葛[2]; Jingxua Hou[1]

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The medium-low maturity shale reservoir has been paid more and more attention because of its huge hydrocarbon generation potential. In-situ underground conversion technology is considered as a kind of extraction technology that can maximize the utilization of medium and low maturity shale. Compared with atmospheric water and steam, supercritical water has unique physical and chemical properties such as low density, low viscosity, good fluidity and strong organic matter dissolution ability. As a pyrolysis medium for reservoir, supercritical water can dissolve all kinds of organic matter, promote the transformation of organic matter and improve the pyrolysis efficiency. In this study, the supercritical water pyrolysis experiment of Chang 73 medium-low maturity shale was carried out through the self-constructed supercritical water high-temperature and high-pressure pyrolysis experimental device. The evolution of pore structure of shale after supercritical water is systematically analyzed by nitrogen adsorption/desorption and mercury intrusion porosimetry analysis. The results show that after supercritical water treatment, the specific surface area, pore volume and average pore diameter of shale increase significantly. Supercritical water as a pyrolysis medium

is conducive to the development of shale pores. After supercritical water treatment, a large number of unconverted kerogen and undischarged heavy hydrocarbon in the core are cracked into oil and gas products, and escape from the core matrix to form a large number of organic pores. The expansion of pores inside shale and the development of effective pores are conducive to the formation of more seepage channels inside shale, thus increasing the connectivity of shale matrix. The above research results provide an important theoretical basis for the application of in-situ extraction technology of shale supercritical water.

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MS03 / 840

A new multi-level discrete fracture model for multiphase flow in complex multi-scale fractured systems

Author: Longlong Li[1]

Co-authors: Luting Wang [2]; Denis Voskov [3]

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In this study, we present a new version of the multi-level discrete fracture model (MLDFM) for multiphase flow in complex fractured systems with features present at various scales. In MLDFM, two levels of unstructured grids conforming with each other are constructed. In a fine-scale grid, both large and small features are represented in conformal DFM manner, and in a coarse grid, only large fractures are conformable depicted. The small-scale features in a coarse grid are dynamicly upscaled as a third continuum similar to the Dual Porosity Dual Permeability model. The DFM treatment for all fractures guarantees accurate solutions for simulations adopting fine-scale grid but unavoidably increases the computational burden. In this work, we developed a computational framework, where the conformal DFM is used to capture the small-scale flow response and homogenize it to the coarse-scale unstructured model applied for forward simulation. An adaptive local-global upscaling formalism is employed to couple the two scale solutions. In detail, we generate local boundary conditions in the fine-scale domain following the basis function interpolation approach and subsequently resolve the flow response. Then, we update the transmissibility for the triple continuum model through the dynamic flow-based upscaling method. Finally, we test the MLDFM approach for several realizations of complex multi-scale fracture systems against fine-scale solution, The simulation results demonstrate the exceptional accuracy and performance of the proposed method.

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MS03 / 841

Bubble growth and induced flow characteristics in porous media under heating conditions

Authors: Zhi Feng[1]; kailun Zhang[1]; Jinqing Wang[1]; Peng Xu[1]; Rui Wu[2]

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The release of trapped bubbles from dead-end porous media filled with nonvolatile liquid holds extensive applications in gas–liquid reactors, CO2-assisted srteam flooding, ceramic sintering, and droplet microcarriers. Since traditional pressure-driven flow fails to induce bubble transport in dead-end pores, this study investigates the potential use of heating to control the release of bubbles from dead-end porous media. This study addresses the issue of bubble retention in dead-end porous media and designs various microfluidic chips with different porous structures, including upward sparse and downward dense, upward dense and downward sparse, and isotropic porous media. The porosity of the sparse and dense regions is 0.7355 and 0.8718, respectively. Using CO2 as the gas and dimethyl silicone oil as the liquid, a self-built Micro-PIV visualization experimental system is employed to investigate the influence of porous media pore structures on the growth and release of bubbles, as well as the induced flow field patterns under heating conditions. The results show that an increase in temperature leads to the transfer of dissolved gas to the bubble, resulting in an increase in bubble pressure, which serves as the driving force for the bubble to pass through the pore throat. Under heating conditions, changes occur in the surface tension of the gas-liquid interface and the viscosity of the liquid phase, while capillary pressure is a key factor for the bubble to pass through the channel. Blockage occurs when the bubble interface capillary pressure is less than the threshold pressure and breakthrough happens when it is greater. The structure of porous media with dense upper and sparse lower regions impedes bubbles from entering low porosity zones, reducing the coalescence probability. Conversely, the structure with sparse upper and dense lower regions increases the coalescence probability, facilitating bubble expulsion. When bubbles seal pores, their continuous growth causes the liquid velocity of corner film flow to rise. During bubble release, the surrounding liquid accelerates to fill the original space, causing a simultaneous transition that induces vortices along the microcolumn walls.

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MS18 / 842

Assessment of colloidal gas aphrons stability for soil remediation: experiments and molecular dynamics simulations

Authors: Ayaulym Amankeldiyeva[1]; Samal Kaumbekova[1]; Yerlan Amanbek[2]; Stéfan Colombano[3]; Yanwei WANG[1]; Sagyn Omirbekov[1]

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Colloidal gas aphrons (CGAs) are layered microbubbles with sizes between 10 and 100 μm and a gas fraction of 40-70% 1. CGAs can enhance contaminant removal from soil and aquifers due to their low environmental impact, high surface area, versatility, and stability as an alternative to surfactant solutions and conventional foams. Hence, it can physically remove organic contaminants and heavy metals and deliver chemical additives, microorganisms, and oxygen to polluted zones 2.
Prior studies have investigated CGAs' stability and the effect of surfactant-polymer concentrations, salinity, and the impact of stirring rate and time were previously studied at the bubble scale [3], [4]. However, a complete understanding of CGAs' stability and the effect of various physicochemical processes on stability at the interface, specifically at the molecular level with and without contaminants, still needs to be made clear. In addition, understanding the relationship between the interaction of molecules and bubbles requires further elucidation.
This study aims to address the knowledge gap by performing experimental research on the stability of CGAs at a bubble scale and the impact of various surfactant-polymer concentrations. Additionally, to numerically investigate the interactions between CGA components at the atomic level via molecular dynamics (MD) simulations.
The experimental process involves generating CGAs using a base fluid designed by a specific concentration of xanthan gum (XG) polymer in demineralized water by mixing with a digital overhead stirrer at 8000 RPM for 20 minutes [5]. Then, a concentration of sodium dodecyl sulfate (SDS), a surfactant, was added to the base fluid and mixed at the same rotation speed for two minutes to generate CGAs. We performed CGAs with various concentrations for the surfactant (1–10 CMC) and polymer (1000–10,000 ppm). CGAs' bubble size variation was investigated using a Zeiss digital microscope with a charge-coupled device (CCD) camera [6]. The images were analyzed using "ImageJ" software to determine bubble size distribution as a function of time. MD simulations are conducted based on similar surfactants, polymer segments, and water fractions using the GROMACS software.
As a result, the concentration of polymer and surfactant are the main factors affecting the stability of CGAs. At polymer concentrations starting from 6000 ppm, optimal stability and a decrease in bubble size are observed. As the polymer concentration increases, the effect of surfactant concentration on the size distribution of CGA bubbles decreases. As polymer concentration increases, smaller bubbles result from decreased air penetration caused by increased base fluid viscosity. Moreover, MD simulations revealed the intermolecular interactions among polymer segments, surfactants, and water molecules and the detailed interfacial structure. This study concluded that selecting the optimal

concentrations of the polymer and surfactant is necessary based on the results of bubble stability testing and MD simulations.

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MS06-A / 845

Modeling of Gas Chimney Formation During Geological Storage

Author: Lyudmila Khakimova[1]

Co-authors: Yury Alkhimenkov [2]; Yury Podladchikov [3]

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Fluid-rich chimney-like structures characterized by a high porosity and permeability are widely observed in sedimentary basins. Thus, understanding the mechanisms leading to focused fluid flow is crucial in predicting natural and human-induced fluid leakage, especially in geological sequestration scenarios. Mechanical and reactive porosity waves provide a mechanism predicting spontaneous localization of fluid flow within sedimentary, without relying on predefined flow pathways and fracture structures.

In this study, we have developed a coupled hydro-mechanical model that allow to predict the spontaneous localization and wave-like propagation of porosity anomalies leading to spontaneous formation and evolution of high-permeability channels through lithological boundaries with sharp properties contrasts. The governing equations describe the filtration of pore fluid in deforming viscous-

elasto-plastic matrix. The proposed model considers the generation of (de)compaction-driven leakage pathways. We also consider the extension of the model to estimate the effect of reactive fluid flow on leakage pathways formation. Our numerical implementation relies on Matlab prototype and GPU-based code using the CUDA-C programming language to resolve flow localization and channels formation on high resolution solving the coupled hydro-mechanical model at reservoir scales. Our results provide numerical predictions of fluid-rich chimney formation during geological sequestration for different rheological types of rocks and lithology layers. Results are shown as an application to the Tornerose and the Snøhvit field in the South-West Barents Sea, and seismic imaging is used as a proxy for chimney comparison.

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Poster / 846

Petrophysical Properties Estimation Based on Digital Rock Modeling for Sandstone

Author: Lyudmila Khakimova[1]

Co-authors: Andrey Morkovkin [2]; Alexander Burukhin [2]; Alexey Cheremisin [2]

[1] *University of Lausanne; Skoltech Institute of Science and Technology*

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Permeability and capillary pressure curve are important to characterize hydrocarbon-bearing formations. There are several laboratory approaches to estimate such petrophysical properties. Nevertheless, one faces with the range of complications such as uncertainties during laboratory measurements, treating micro- and nano-pore permeability and multi-scale geometry of the pore space, complex mineral composition.

Within this work, to provide petrophysical properties prediction we combined laboratory investigation and one- and two-phase fluid flow simulations using digital rock models. The workflow was applied for low permeable samples from sandstone reservoir with measured complex mineral composition. We utilized the combination of high-contrast μCT scanning technique and Focused Ion Beam milling with Scanning Electron Microscopy (FIB-SEM) to construct high quality 3D multiclass digital rock models of sandstone samples. The constructed 3D multiclass digital rock models were used as an input for simulations of one- and two immiscible fluid flow through such 3D multiclass porous media and further analysis. Numerical approaches include the direct Navier-Stokes, the Lattice Boltzmann methods. Permeability and drainage capillary pressure curves were experimentally determined from laboratory measurements on core samples and compared to the simulation results. Both predicted permeability and drainage capillary pressure curves were in a good agreement with experimental values.

Acknowledgments: Authors thank the Ministry of Science and Higher Education of the Russian Federation under agreement No. 075-10-2022-011 within the framework of the development program for a world-class Research Center.

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MS10 / **848**

Non-invasive imaging of solute redistribution below evaporating surfaces using 23Na-MRI

Author: Mohammad Ali Chaudhry[None]

Co-authors: Andreas Pohlmeier [1]; Johan Alexander Huisman [2]; Rainer Helmig [3]; Stefanie Kiemle

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Evaporation from porous media is a key phenomenon in the terrestrial environment and is linked to accumulation of solutes at or near the evaporative surface. Such accumulation eventually leads to salinization, soil degradation and weathering of building materials, topics with high economic impacts. A thorough understanding of evaporation and the associated solute accumulation requires the development of physical models describing the most relevant processes and their validation by experiments.
In this context, the current study aims at the understanding of solute accumulation near evaporating surfaces for model porous media at the cm-scale. Analytical and numerical modelling predict the development of local instabilities due to density differences during evaporation in case of saturated porous media with high permeability, which eventually causes density-driven backflow through fingering [Bringedal et al. TPM 2022]. To experimentally investigate this process, we performed evaporation experiments on sand packings with a diameter of 3.1 cm and a height of 4.0 cm prepared with two types of porous media with 1 M NaCl solution: F36 (medium sand) and W3 (fine sand/silt) with porosities of 0.37 and 0.39, respectively. The intrinsic permeability of the two packings differed by two orders of magnitude, i.e. 2.9×10-11 m2 for F36 and 5.6×10-13 m2 for W3. Using magnetic resonance imaging (23Na-MRI), we monitored the development of solute accumulation and subsequent backflow with high spatial (1 mm) and temporal (1 hr) resolution during evaporation with a continuous supply of water at the bottom of the samples (wicking conditions).
Significant differences between the 23Na enrichment patterns were observed for the two types of sand. F36 sand produced an initial enrichment at the surface within the first hour, but soon after a downwards moving plume developed, hence redistributing NaCl back into the column. This was

attributed to density driven backflow made possible by the high permeability. The backflow caused a good mixing of the solute during the observation period of 120 h. 1D concentration profiles with depth obtained from the 3D MRI imaging showed that the average concentration reached only 2.5 M, well below the solubility limit of 6.13 M. In contrast, for fine W3 sand with lower permeability, enrichment only took place in a shallow near-surface zone of a few mm with a maximum concentration of 5.1 M after 73 hours of evaporation. No fingering occurred although the mean evaporation rate was similar to that of the F36 sand. These results highlight the major role that porous media properties play in solute redistribution near evaporating surfaces, which was predicted by theory and now confirmed experimentally. The findings encourage further investigations involving different porous media with systematic variation of hydrological properties and the coupling of experimental results to numerical modelling.

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Poster / 849

Numerical simulation of yttrium oxide grain sintering

Authors: Dmitry Prokhorov[1]; Eugene Malkovich[1]; Vadim Lisitsa[2]; Vladimir Derevshchikov[1]; Yaroslav Bazaikin[3]

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Yttrium oxide is a promising and poorly studied material for the field of catalysis. It can be used as a support in catalytic processes such as carbon dioxide reforming of methane and CO_2 methanation. Predicting changes in the texture of Y_2O_3 during temperature treatment is an important material science and a computational task.

In this study, we applied a phase-field approach to obtain an accurate mathematical description of Y_2O_3 sintering over a wide temperature range. The general principle of the phase-field method is to describe physical quantities by a set of continuous fields that take constant values in specific regions and smoothly change in the interfaces between these regions. In the case of sintering, such areas are the individual grains of the material. The interface of the microstructure has a finite width along which the sintering materials move. The Allen-Cahn and Cahn-Hilliard equation system is used to describe changes in order parameters and mass density distribution.

To verify the mathematical model, yttrium oxide sintering experiments were carried out and data on the textural and structural properties of Y_2O_3 were obtained. The developed model makes it possible to calculate the decrease in the specific surface area and pore volume of yttrium oxide for pores ranging from 3 to 70 nm and determine the growth rate of Y_2O_3 crystallites during sintering. The model allowed us to determine that stepwise heating from 600° C to 900° C and then 1200° C decreases the specific surface area of yttrium oxide from 54 m^2/g to 15 m^2/g and then to 5 m^2/g, respectively.

It should be noted that the obtained experimental micrographs of the cross sections of yttrium oxide samples are in visual accordance with the model images. The approach used in work can be used to predict the evolution of the textural properties of porous materials (catalysts, sorbents, ceramics) under high-temperature conditions.

The study was carried out with funding provided by Russian Science Foundation grant number 21-71-20003

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Study on the law of enhancing CO2 displacement effect and reducing oil-gas miscible pressure by surfactant

Authors: Gaoyu Li[1]; Lei Li[1]; Mingjian Wang[1]; Yongmao Hao[1]; Yuliang Su[1]; Zheng Chen[1]; Zirui Fan[1]

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CO2 flooding technology is currently one of the most promising methods for enhancing oil recovery in unconventional reservoirs, but it is difficult to achieve CO2 miscibility under most reservoir conditions. Oil and gas contact in large pores is mostly a single contact, and only a small amount of CO2 is dissolved in crude oil, which is difficult to fully play the role of CO2 in increasing expansion and reducing viscosity, and it may even be too late to extract light hydrocarbons.As a result, it is difficult to form the displacement belt, the breakthrough time is too early, and the ultimate oil recovery can not achieve the requirement. As a material to reduce the interfacial tension between different media, the surfactant can solve the above problems.Aiming at the study on the law of low permeability reservoir surfactant enhancing CO2 displacement effect and reducing oil and gas miscibility pressure, the porous medium fine tube microfluidic chip which can replace the fine tube in macro fine tube experiment was prepared. Five ultra-low interfacial tension surfactant, including ethylene glycol buether, Span-80 and mixed styrene, viscosity reducing agent KD-45A and agent HA007F, were selected.The effect of various agents on reducing the miscible pressure of CO2 and crude oil was studied, and the effect of high temperature and high pressure interfacial tension disappearance method was used to evaluate the interfacial tension of CO2 and crude oil respectively.The

experiments include the suspended drop method to measure the interfacial tension at 70℃ and atmosphere pressure, and the high temperature and high pressure microfluidic experiment at 100℃ and 20-50MPa. The results show that adding 0.3% mass concentration reagent to crude oil can effectively reduce the interfacial tension of oil and gas, and with the increase of gas injection pressure, the solubility of CO2 in crude oil increases, the degree of miscibility increases, more light hydrocarbons are extracted, and the oil displacement efficiency can be improved.Among them, ethylene glycol butyl ether, Span-80 and HA007F agents are the most effective, because at the front end of the oil-gas contact, the crude oil will be bound to the lipophilic functional group of the surfactant, and the other end, the CO2-philic end, will be bound to CO2 gas. In this way, the polar difference between crude oil and CO2 will be reduced, the interfacial tension will be reduced, and the macro performance is that the three phases of oil, gas and surfactant are mixed together to form a miscible oil displacement belt, which not only enhances the diffusion rate of CO2, strengthens the mass transfer behavior and extraction rate of oil and gas interface, but also significantly reduces the miscible pressure of CO2 and crude oil, so that the degree of crude oil use will be greatly increased.

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Study on the Microscopic Residual Oil Distribution State and Dynamic Utilization Mechanism of Gas-Driven Remaining Oil in Sandstone Reservoirs

Authors: Dian Zhang[1]; Hongwei Niu[1]; Jiarui Sun[1]; Yuliang Su[1]; Zheng Chen[1]; Zihan Hou[1]; lei li[1]

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The pore-throat structure of the sandstone reservoir in Xinjiang is mainly composed of intergranular pores and intragranular dissolved pores. The overall permeability conditions deviate, with a clay mineral absolute content of 2.93%, indicating a moderately weak water sensitivity. The reservoir exhibits strong heterogeneity, and the state and mechanisms of residual oil after gas injection are complex, limiting the effectiveness of reservoir development. In this study, the pore distribution of rock cores was evaluated through high-pressure mercury injection. Gas displacement experiments, combined with Nuclear Magnetic Resonance (NMR) technology, were used to quantitatively characterize the gas-driven residual oil distribution at different pore-throat scales. The study analyzed the dynamic mechanisms of residual oil under different gas injection conditions. The results indicate that gas injection can alter the distribution pattern of oil phases in sandstone, effectively displacing residual oil. The recovery efficiencies with different injected gases (such as CO2, CH4, N2) were 40.54%, 37.76%, and 33.6%, respectively. Among them, CO2 primarily utilizes a mixed-phase displacement-dissolution expansion mechanism, affecting nano-scale pores, especially micro and small pores. The

recovery contributions are mainly from medium to large pores with a radius greater than 0.1 μm, accounting for 93.29% and 99.71%, respectively. CH4 utilizes a mixed-phase displacement-dissolution extraction mechanism, affecting nano-scale pores, with recovery contributions mainly from medium to large pores with a radius greater than 0.1 μm, accounting for 79.21% and 97.19%, respectively. N2 shows significant effects on medium to large pores, with minimal impact on micro pores. The recovery contributions from medium and large pores are 70.18% and 85.07%, respectively, while the recovery contribution from micro pores is only 3.01%. Increasing the injection pressure from 30 MPa to 40 MPa resulted in a 15.8% increase in crude oil recovery. Simultaneously, the water cut increased from 20% to 60%, leading to a reduction of around 20% in gas-driven recovery efficiency.

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MS17 / 854

Investigation of the Effect of Thermal Stresses on Hydraulic Fracturing in Geothermal Reservoirs

Author: Abolfazl Ghadimi[1]

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Geothermal energy has been widely proposed as a potential green energy resource to replace traditional fossil fuels. The most ubiquitous form of geothermal energy is found in hot dry rocks which are usually composed of granite (or other types of volcanic rocks) with very low permeability and are developed as enhanced geothermal systems (EGS). Hydraulic fracturing is a powerful technology to increase the permeability, enhance the water –rock contact and maximize the economic potential of EGS.

Due to the high cost associated with hydraulic fracturing operations, it is important to build reliable tools for predicting how the formation will respond to water injection. Numerical modeling of hydraulic fractures is an important method for studying fracture parameters such as length, width and fluid leak-off. In enhanced geothermal systems, the typical temperature difference between the reservoir and the injected fluid can range from 200◦C to 300◦C. As a result, the injected fluid rapidly cools down the near wellbore area and the resulting thermal contraction generates thermal tensile stress. This stress reduces fracture breakdown and extension pressure. Increase in injectivity near injection wells resulting from thermal contraction has been reported by researchers [1, 2] at the beginning of the injection process.

Hydraulic fracturing is widely used for improving permeability in hydrocarbon reservoirs [3], hazardous solid waste disposal [4, 5], for leaching processes and fault reactivation in mining [6], and soil and groundwater remediation [7] as well. The studies have shown that even for such non-geothermal applications, cryogenic effects help to reduce the water consumption, formation damage, and the environmental impact of water-based fracturing [8].
Modeling of thermal stresses in hydraulic fracturing requires coupling of hydro-thermal physics with fracture mechanics. In this study, a more accessible method than developing a complex finite element code for this purpose has been proposed. Hydraulic fracturing was modelled by creating a three-dimensional model using Abaqus software, and thermal effects were incorporated using heat-sink boundary conditions. The results were validated against analytical and experimental studies. Investigation of the influence of thermal properties of rock and the hydraulic fracturing design parameters, on fracture geometry and pressure showed that the temperature difference between rock and injected fluid, thermal expansion coefficient of rock, and thermal conductivity of rock are the most significant factors in defining hydraulic fractures'geometry and fracking pressure in geothermal reservoirs. In general, hydraulic fractures exhibit greater opening and less extension under thermal stresses compared to non-thermal fracturing processes.

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Poster / 857

Unlocking the secrets of unconventional shale: A multi-scale approach to understanding fluid transport and resource recovery

Author: Yeping Ji[1]

Co-authors: Andrzej P. Radlinski [2]; Chen Xiao [1]; Claudio Delle Piane [1]; Klaus Regenauer-Lieb [3]; Mihaela Grigore [1]; Phung Vu [2]; Tomasz Blach [2]

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Understanding the intricate pore structure of shale rocks across scales, from nanometres to micrometres, is crucial for optimizing the recovery of natural gas, geothermal energy, and potentially enabling future CO2 sequestration and subsurface hydrogen storage. This study leverages Small Angle Neutron Scattering (SANS), a non-destructive technique, to precisely characterize pore properties in Australian shale samples. By employing contrast matching experiments, we probe the accessibility of these pores to deuterated methane (CD4).
Our in-situ SANS experiments, conducted on carefully chosen shale samples with diverse thermal maturities and organic carbon contents, reveal how stress and fluid pressure influence the overall pore structure. Notably, we observed that:
• Nanopore gas confinement exhibits sample-specific behaviour.
• Applying pressure to methane (CD4) at 500 bar induces condensation within accessible nanopores (diameter < 10 nm), resulting in the scattering length density (SLD) of confined methane exceeding that of the shale matrix by more than twice.
• Uniaxial stress, mimicking hydraulic fracturing pressure, enlarges some smaller pores and potentially even forms larger ones through coalescence, while expelling confined methane.
These findings provide valuable input for advanced modelling and simulations, enabling us to bridge the gap between submillimeter-scale laboratory data and reservoir-scale behaviours. This paves the way for optimizing resource extraction and developing novel strategies for geological storage of critical elements.

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MS19 / **858**

Analyzing uncertainties of the instability of the anode /electrolyte interface in solid state batteries

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Modern batteries must meet stringent performance standards to qualify for use in technological solutions that seek to address current global environmental challenges. Such batteries should exhibit high energy densities, fast charging, and long cycle lives while maintaining a high degree of safety. Solid-state batteries (SSBs) exploit high-capacity anode materials such as Lithium or Sodium metal and are expected to deliver high standards that meet the stringent needs of long-range electric vehicles and large-scale renewable energy storage. However, stability in these devices presents important challenges. The interface anode/electrolyte interface is home to structural imperfections that lead to heterogeneous stripping and plating during cell cycling, significantly reducing cell capacity and compromising cell safety. Although numerous studies have attempted to shed light on the root causes of inhomogeneous electrochemical processes at metals anodes in SSBs, the detailed atomistic processes that lead to ubiquitous dendrites growth in metal anodes are not well elucidated. Critically lacking is the detailed understanding of the thermodynamic driving forces that lead to such degradation at the atomistic level.
We analyze the forward propagation of the imperfection parameters that are susceptible to highly defeat the stability of the anode/electrolyte interface. The imperfections in inputs are parametrized as random variable and Monte Carlo method and sensitivity analysis approaches allow a better understanding of Lithium plating and stripping behaviors.

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MS07 / 859

Multiscale Extended Finite Element Method for the Simulation of Fractured Geological Formations

Author: Fanxiang Xu[None]

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In the prevailing context of the 21st century, characterized by a predominant reliance on oil and gas, or in the promising future where green energy shapes a human society committed to net-zero emissions, the role of underground fractured formations in energy production (geothermal) and storage remains pivotal and irreplaceable. In the past decade, hazardous consequences of failing to predict the geomechanics behaviors of fractured formations has led to a pronounced focus on developing simulation strategies that are both accurate and efficient for subsurface fractured formations.
As a widely used simulation method in fracture mechanics, the extended finite element method (XFEM) provides a precise approach to simulate deformation and fractures propagation within highly fractured media. It is also a convenient strategy as it allows for the use of structured grids. However,

the expensive computational cost of using classical XFEM in the simulation of fracture networks makes this method not immediately suitable in the geoscientific community.
To resolve this challenge, a multiscale extended finite element method (MS-XFEM) is proposed to provide a novel approach to simulate the highly fractured subsurface formations accurately and efficiently. The deformation and fractures propagation are both simulated by interpolating the solutions from a larger yet sparser coarse grid to the original fine-scale grid. This interpolation process requires the construction of the basis functions matrix. The novelty of this work is to involve the fractures into basis functions only, thus the coarse scale system is constructed based on a standard finite element method. More importantly, this construction of basis functions is fully algebraic and can be updated locally and adaptively for the simulation of propagating fractures. This method has been implemented and tested to prove its efficiency and accuracy. All test results prove the good qualities of solutions computed from MS-XFEM when compared to fine scale XFEM solutions. Basis functions are constructed successfully with the algebraic method since they capture all different types of discontinuities. These tests reveal the potential of MS-XFEM in simulating real-world subsurface fractured formations.

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Poster / 860

Covalent Organic Frameworks Supported Highly Active Fe-N-C Catalyst Boosting Oxygen Reduction in Direct Formate Fuel Cell

Author: Linghan Lan[1]

Co-authors: Yaxing Zhu [1]; Guangfu Liu [1]; Juchao Liang [1]; Ping Zhang [1]

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Direct liquid fuel cells have become an ideal power source for rapidly emerging miniaturized and portable electronic products due to their advantages of cleanliness, environmental friendly, high efficiency, safety, long endurance, and fast “charging”. However, at present, the cathode catalysts for oxygen reduction reaction (ORR) of such fuel cell are still mainly platinum or platinum-group noble metals, which leads to the high cost. In addition, these precious catalysts may be poisoned and inactivated during the operation of the fuel cell, seriously affecting the output performance and stability.

In recent year, covalent organic frameworks (COFs) have emerged as a potential materials for energy storage and electrochemistry conversion due to their high porosity, atomically precise structures and designable topological architectures. Thus, COFs material was synthesized in this study to serve as the support for FePc by facilely sovolthermal process, forming highly active Fe-N-C catalyst to boost ORR in direct formate fuel cell (Fig. 1a). Different load of FePc into COFs (Fig. 1b) was investigated and one could see that the most active COFs-supported catalyst (FePc1@COFs5) exhibited higher onset potential of 0.929 V (vs. RHE) and half wave potential of 0.862 V (vs. RHE) than that of commercial Pt/C (0.928 and 0.845 V (vs. RHE)) (Fig. 1c). Further, the direct formate fuel cell with FePc1@COFs5-coated cathode also archived higher power density and limiting current than that with Pt/C catalyst (Fig. 1d). The facile synthesis process and high performance of COFs-supported catalyst broaden the development for COFs application in electrochemistry energy conversion.

Fig. 1 (Seen in attachment) (a) Schematic illustration of membrane-free direct formate fuel cell with Pd-deposited Ti mesh anode and COFs-supported catalyst-coated air cathode, (b) Fe content in different samples, (c) Linear sweep voltammetry scanning for different samples in 0.1 M KOH by scanning rate of 10 mV/s, (d) power density curves of membrane-free direct formate fuel cells with 2 mg/cm2 Pt/C-coated cathode and 2 mg/cm2 COFs-supported catalyst-coated cathode.

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MS13 / 861

Molecular Simulation of Competitive Adsorption of H2S-Containing CO2 and CH4 in Organic and Inorganic Shale Nanopores

Author: Jingkai Cui[1]

Co-authors: Junyao Bao [1]; Shaofeng Ning [2]; Shiyuan Zhan [1]; Xiaoguang Wang [1]

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Objectives/Scope:
Geological storage of acidic gases can reduce atmospheric emissions of CO2 and H2S, thus serving as a critical part of low-carbon energy systems. Depleted shale gas reservoirs are good storage candidates owing to their intrinsic gas storage capacity. However, shales exhibit complex structural characteristics and abundant micro- and nano-scale pores, where gases primarily adsorb. Consequently, comprehending gas adsorption mechanisms in shale nanopores is imperative for shale gas geological storage. In this

*study, we simulated CO2, H2S and CH4 adsorption in organic/inorganic shale nanopores under various pressures using grand canonical Monte Carlo (GCMC) simulations. We calculated their adsorption quantities and selectivity coefficients under assorted conditions and analyzed competitive adsorption. This work elucidates shale gas adsorption from a molecular perspective and lends insights into storage assessments.*Methods/Procedures/Process:
We constructed molecular models of shale nanopores with diverse structures, encompassing hydroxylated quartz nanopores and graphitic organic nanopores. We examined CO2, H2S and CH4 adsorption in these pores under various pressure conditions (373.15K). The molar ratio of CO2, H2S and CH4 was fixed at 4:1:5. CLAYff and Steele 10-4-3 potential models described quartz and graphite correspondingly, while the TraPPe and Nath force field models represented CO2/CH4 and H2S individually. Component densities and chemical potentials were computed based on gas composition. CO2, H2S and CH4 insertions, translations and rotations were conducted over 20 million MC cycles, equalizing pore gas chemical potentials to calculated values. The first 12 million cycles achieved chemical potential equilibrium, and the subsequent 8 million cycles collected gas distribution data. The Langmuir-Freundlich adsorption model fitted the isotherms. Competitive gas adsorption was examined by quantifying adsorption quantities and selectivity coefficients.
Results/Observations/Conclusions:
*Gas adsorption capacities were superior in organic versus inorganic pores across all gases examined. Graphite ostensibly furnished additional adsorption sites, whereas hydrogen sulfide and carbon dioxide occupied further sites in quartz nanopores. Therein, CH4 adsorption selectivity was markedly inferior to CO2 and H2S. Excess CH4 adsorption approached 0 as pressure rose, however excess CH4 adsorption in organic pores increased with pressure. H2S displayed the maximal adsorption selectivity coefficient universally, imprinting the strongest competitive adsorption capacity, which intensified in organic nanopores. Under certain quartz pore conditions, CO2 adsorption selectivity closely approximated H2S and exceeded CH4 substantially, unveiling comparable CO2 and H2S competitive adsorption capacities in inorganic pores given natural gas presence in reservoirs.*Applications/Significance/Novelty:
This study elucidates the competitive adsorption between acidic gases and natural gas in depleted shale gas reservoirs from a molecular vantage, thus facilitating augmented comprehension of CO2/H2S adsorption mechanisms in natural gas-laden formations while steering acidic gas geological storage in shale.

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Poster / 867

AI assisted prediction of Sweep Efficiency of Hydrogen –Water Displacements in Porous Media

Author: Amirsalar Manouchehri[1]

Co-author: Mozhdeh Sajjadi [2]

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In the present era of escalating global energy consumption, there has been a marked shift in the dynamics of energy supply and demand, resulting in significant disparities between these two variables throughout the year. To address this imbalance, energy storage technologies have emerged as a potential remedy to facilitate the integration of renewable energy sources. Among these technologies, underground hydrogen storage has received considerable attention as a viable option for large-scale energy storage. Hydrogen can be stored in various subsurface structures, including aquifers, depleted oil and gas reservoirs, and salt caverns. Aquifers, defined as layers of permeable and porous rock containing fresh or saline water at considerable depths, are widespread in sedimentary basins worldwide. Therefore, exploring the potential of utilizing aquifers for hydrogen storage may help overcome the geographical constraints associated with alternative storage options.

The retrieval of stored hydrogen is a critical consideration that can significantly impact feasibility assessments and performance projections of the storage process. Factors such as hydrogen dilution with cushion gas, chemical reactions, and entrapment within the aquifer can lead to reduced hydrogen recovery. These phenomena are influenced by pore structure, interfacial properties between hydrogen and water, and flow dynamics.

Accurate modeling of the injection-production cycles to estimate the residual hydrogen saturation, and consequently the recoverable amount of hydrogen, necessitates time allocation and multi-phase flow parameters, often unavailable. As a result, machine learning methods have been explored for sensitivity assessment and displacement efficiency estimation. In this study, a machine learning approach was employed to predict the sweep efficiency of hydrogen –water displacement in synthetically designed porous media.

To achieve this objective, artificial porous environments with varying particle size distributions and random spatial arrangements were generated and incorporated into the simulation software. A numerical model was developed to simulate displacement processes within these environments. The simulation results, including the image of the porous medium, and the parameters defining the displacement scenario such as injection rate, fluid properties, and interfacial characteristics, were utilized as input data to the algorithm. During the training phase using machine learning, two approaches based on image processing of the porous medium—Multi-Layer Perceptron (MLP) and Convolutional Neural Network (CNN)—were employed. The primary goal of both algorithms was to predict displacement performance and saturation profiles within the porous space. The results show the aptness of these algorithms for prediction of recoverable hydrogen in terms of the porous medium's description and two-phase flow parameters.

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Hydrogen Capillary Trapping and Hysteresis in Sandstone - A Core Scale Study

Author: Omid Shahrokhi[1]

Co-authors: Nikolaos Diamantakis [1]; John M. Andresen [1]; M. Mercedes Maroto-Valer [1]

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Hydrogen is a low-carbon fuel that has the potential to contribute to the large-scale decarbonization of different sectors, including power generation, heating, transportation, and industry. Blending hydrogen into national gas distribution networks can also help decarbonize distributed carbon emissions from domestic consumers where carbon capture is not feasible. However, the reliable and robust operation of a gas network at the national scale would critically require safe and efficient large-scale hydrogen storage. For example, to meet the UK's seasonal demand and production variations from intermittent renewable energies, 0.37-1.58 billion cubic meters of hydrogen storage capacity is required, representing 25-105% of the current UK strategic natural gas storage capacity 1. This means large-scale repurposing of current storage sites (salt caverns and depleted gas reservoirs) and developing new sites.

To increase confidence in the large-scale storage of hydrogen in depleted gas reservoirs and saline aquifers for efficient hydrogen storage, understanding the multiscale flow and trapping mechanisms of hydrogen is critical. As part of a comprehensive study, cyclic flow experiments of hydrogen in the Sherwood sandstone reservoir at pore and core scale were performed. Here we share the results of cyclic core scale flow experiments we performed at reservoir conditions (108 bars and 50℃). Three sets of flow experiments were conducted. Experiment 1, started with rock fully saturated with H2 and continued for eight injection periods of alternating hydrogen and brine. A similar sequence of fluids was injected in Experiment 2, however, the injection started with the core fully saturated with synthesized formation brine. Experiment 3 was performed to check the repeatability of Experiment 1. In this experiment, four injection periods were considered sufficient.

These experiments are designed to explore hydrogen capillary trapping and relative permeability hysteresis during cyclic fluid displacements representative of seasonal storage and production of hydrogen in subsurface reservoirs. The choice of experimental conditions as well as rock sample and brine composition were informed by wellbore logs provided by the British Geological Survey. The rock sample selected was Sherwood sandstone with high porosity (~28.5%) and permeability (~700mD). The mineralogy of the rock type ensured negligible geochemical reactivity with hydrogen (e.g., the lack of FeS2 - pyrite). This helped us isolate the active trapping mechanisms of capillary forces. To ensure gravity-stable fronts, hydrogen is injected from the top and brine from the bottom of the core holder. The alternate injection of hydrogen and brine is then performed until no significant change in saturation is observed along the sample (typically 2 pore volumes except for the first injection period where injection rates were ramped). During each injection period, pressure drops along the core, hydrogen and brine production and injection rates are monitored. This data was then used to calculate the average hydrogen saturation and trapped quantity after each brine injection. The production data is history matched with a compositional model to allow measurement of flow functions. Hysteresis of relative permeability was observed in all experiments. The change in flow function trends and trapping provided reliable input to our reservoir scale model.

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Insights into Salt Precipitation Dynamics during CO_2 Storage in Saline Aquifers: A Pore-Scale Perspective

Author: Puyan Bakhshi[1]

Co-authors: Omid Shahrokhi [1]; Mercedes Maroto-Valer [1]

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The escalating challenge of global warming has intensified the pursuit of effective carbon management strategies. In this context, underground CO_2 sequestration, particularly in deep saline aquifers, emerges as a promising solution, offering a safe and substantial storage capacity for captured carbon emissions. This study provides an in-depth pore-scale investigation into the phenomenon of salt precipitation during CO_2 storage in saline aquifers, a critical factor affecting the efficiency and sustainability of CO_2 sequestration.

Our research embarked on an extensive exploration of the processes and impacts of salt deposition within pore spaces, which occurs when CO_2 is injected into saline aquifers. This deposition is capable of altering the petrophysical characteristics of the formation rock, potentially decreasing permeability and triggering pressure build-ups, thereby impeding the CO_2 injection process. To address this, we developed a sophisticated high-pressure, high-temperature μ-CT core flood experimental apparatus. This setup, featuring an X-ray translucent core holder, facilitated in-situ 3D imaging of flow dynamics under conditions resembling those in natural subsurface environments.

We meticulously studied the structural changes in a Doddington sandstone sample, saturated with a highly saline brine, under conditions that simulate typical saline aquifers (90 bar and 50℃). The use of μ-CT imaging allowed us to observe the precipitation mechanisms and assess their impact on the pore structure and flow dynamics within the rock. This investigation revealed a significant porosity reduction, particularly around the injection point, leading to a substantial decrease in the effective CO_2 permeability of the sample.

In addition to structural analyses, our study delved into the primary forces driving salt precipitation within the pore spaces. The interaction of viscous displacement, evaporation, and capillary movements dictated the drying patterns, which are integral to pinpointing the locations of salt accumulation. Notably, while some regions exhibited a decline in effective CO_2 permeability, others showed an increase due to the formation of new CO_2 pathways as a result of brine evaporation.

Our results indicated a general reduction in porosity by up to 11% from the initial value. This decrease, although seemingly moderate, had profound implications for the CO_2 storage capacity of the rock sample. The time-series analysis of the sample's internal structure uncovered a non-uniform salt distribution, with pronounced accumulation near the inlet. This heterogeneity in salt distribution is particularly crucial for understanding and predicting CO_2 injectivity over time.

Furthermore, the study brought to light the dynamic nature of salt redistribution within the pore space. Under the influence of the CO_2 drag force, precipitated salts tended to migrate, accumulating within pore throats and potentially impacting the long-term efficacy of CO_2 storage.

In conclusion, our research offers a comprehensive pore-scale perspective on the dynamics of salt precipitation during CO_2 storage in saline aquifers. The insights gained from this study are instrumental in enhancing our understanding of subsurface CO_2 storage mechanisms.

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MS01 / **877**

Effect of reactive impurities in CO2 gas storage in carbonate reservoirs

Authors: Dmytro Mihrin[1]; Karen Feilberg[2]; Rasoul Mokhtari[1]

Co-authors: Ali Talaei [1]; Komeil Shojaei [1]; Safa Khojamli [1]

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Storage of carbon in the form of compressed CO2 in the subsurface represents a potentially viable and cost-effective way to reduce emission of heat-trapping CO2 to the atmosphere. The feasibility of a CO2 storage scheme depends on many factors, including CO2-induced corrosion and scale; availability of inexpensive CO2 sources, available pipeline, pipeline integrity, temperature and pressure conditions, caprock integrity, biological activity in the subsurface, injectivity, mineral trapping and interactions with the rock surface amongst others. All these factors are potentially affected by the presence of impurities in the CO2 supply. The chemical composition of the CO2 stream will depend on the fuel sources and capture methods, and CO2 with impurities is much more widely available in sufficient quantities for transport to offshore facilities as capture processes and transport generally lead to some content of impurity. The effects of major impurities (SO2, N2 and O2) on phase behavior as well as corrosion in pipelines are quite well understood and widely reported in literature. Some studies have addressed the geochemical effects of impurities on the matrix in the well, mainly for shales and sandstone reservoirs. However, the geochemical effects of long-term storage of impurity-containing CO2 are not well known, particularly for carbonates, including chalk. The theoretical and experimental predictions of the interaction energies for complexes of CO2 with relevant impurities (aminoethanol, ethylene glycol, methanol, ethanol, water, H2S, NH3, CO, NOx and SO2) suggest that the interactions with CO2 vary and some of the species interact strongly even in small quantities compared to small gaseous impurities like N2, Argon and O2. Injection testing of these impurities in Danish North Sea Chalk cores are conducted in core flood experiments combined with chemical analysis of the effluent fluids and chalk surfaces to investigate the alterations caused by impurities.

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Transition from oil & gas drilling fluids to geothermal drilling fluids: Rate of Penetration as bottleneck in geothermal drilling operations

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Co-authors: Daniel Cano Floriano [2]; Igor Paevskiy [2]; Joseph Wee [3]; Mojtaba Mohammadi [4]; Ian Collins [5]

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Geothermal drilling operations are frequently challenging, owing to the harsh downhole conditions encountered in geothermal wells, specifically the high temperatures (HT) together with the toughness of the rock found in many geothermal formations. Drilling in such environments requires specialised drilling fluid formulations that have high thermal stability, good rheological properties, excellent lubricity and low formation damage. In our recently published literature review 1, we have attempted to answer the question: "to what degree can developments in oil and gas drilling fluids be transferred to drilling fluids for geothermal wells?"Here we specifically focus on one key aspect of drilling in HT geothermal formations: the Rate of Penetration (RoP) and the effect of fluid design on RoP. Currently, it is poorly understood how RoP is related to the porous media properties of geothermal rock formations and the maintenance of desirable fluid rheological properties at high temperatures.

To complement our literature research, we analyse the Daily Drilling Reports (DDR) kindly provided by Eden Geothermal 2. The recent drilling campaign in Cornwall used standard oil and gas drilling fluid formulations which resulted in low RoP, accompanied by rapid wear of expensive drill bits and associated increased non-productive time.

The key questions that we have tried to answer are

1. What are the key parameters governing RoP?
2. Does RoP depend on rheology / composition of drilling fluid?
3. Can we make recommendations for new drilling fluid formulations to enhance RoP?

Our review has identified gaps in both fundamental understanding and in existing technology:

1. RoP depends on the rheology / composition of the drilling fluid.
2. RoP increases linearly with decreasing Plastic Viscosity (PV), solid content, and mud weight for both sedimentary and geothermal rock formations.

Furthermore, in agreement with Najjarpour et al. [3], we observe that RoP management has mainly focused on using (semi-)analytical and machine learning models, with several correlations being developed for this purpose.

We provide here, for the first time, a comparison of the field data obtained by Paiaman [4] with the DDR provided by Eden Geothermal 2. Both trends confirm, as identified in our literature review, that RoP decreases linearly with increasing fluid PV and increasing solid content / mud weight.

From these insights we conclude that RoP can be improved using low viscosity and low-density fluids. To address this challenge, we recommend that foams [5] and aphron systems [6] be investigated, as both types of fluid have a low density while showing shear thinning behaviour with increasing shear rate. It should be noted, however, that such systems to date have only been studied at relatively low temperatures and the challenge of increasing the thermal stability of the formulation components needs to be addressed.

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MS15 / **880**

2D to 3D deep learning reconstruction of CO2 electroconversion Gas Diffusion Electrode : a validation study

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Direct 3D imaging of natural or synthetic porosity below ~1µm in diameter often requires the application of Focused Ion Beam Scanning Electron Microscopy (FIB-SEM). This technique has several limitations: high cost and time demands, instrument availability, complex sample preparation and low field-of-view (FoV), restricting its suitability for operational industrial studies. SliceGAN, a generative adversarial network algorithm developed by Kench and Cooper (2021) reconstructs 3D pore space based on a 2D image input (Fig. 1). In conjunction with 2D SEM imaging, SliceGAN has the potential to generate representative porous media images considerably faster and cheaper than FIB-SEM. However, the original work (Kench and Cooper, 2021) did not validate the methodology against 3D images to check whether the synthetic reconstructed media replicate the original porous

materials porosity, permeability, and pore size distributions.
The microporous layer (MPL) of the Gas Diffusion Electrode (Fig. 2), used for the electroconversion of CO2 into ethylene, methanol and other products (Weekes et al., 2018), was selected for the validation of the pore space reconstruction algorithm. Fully resolved images of the MPL porosity are necessary for subsequent modelling of electrode physical properties: permeability, diffusivity and conductivity (McLaughin et al., 2022). For this study, four FIB-SEM validation volumes from two scans at 5 and 10nm resolution and FoV varying from 51 to 94µm3 were analysed. Raw data was segmented, porosity calculated, and permeability of each volume modelled using a steady state single-phase direct numerical simulation in OpenFOAM (Fig. 3). Permeability variation from 4.04e-16 to 8.03e-16 m2 between different volumes is attributed to an insufficient FoV of individual scans, leading to unrepresentative models. A large image aspect ratio, inherent to FIB-SEM scanning, also led to variation of permeability in three principal orientations in the absence of any noticeable material anisotropy.
The open-source network architecture of SliceGAN was adapted to accommodate varying training data crop sizes. Two orthogonal SEM images at 1.7nm resolution and FoV of 315 µm2 were used to prepare training datasets. Ten different studies, combining different crop sizes and input image resolutions, were trained to assess the effect of the 2D training image FoV on the quality of the reconstructed 3D volume. For each study, inference volumes with a maximum FoV of 163µm3, limited by RAM capacity, (Fig. 4) were generated, and their porosities and permeabilities calculated (Fig. 5). While properties vary between studies and between inferences within each study, an overall good match of porosity, permeability, and pore size distributions with FIB-SEM data was observed, with further research to be done on multiphase flow properties of the artificial volumes.
This study shows the verification of the 2D –3D reconstruction algorithm, which, while not creating an exact copy of the real pore space, is able to replicate properties necessary for larger-scale physics modelling. It is also capable of generating significantly larger volumes when compared to FIB-SEM validation data. This, together with the fact that the network is trained on 2D data with a large FoV, addresses the representability issues observed during the FIB-SEM image analysis.

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MS10 / 882

Assessing the Efficacy of Thermal-Sensitive Polymer Gels for Temporary Wellbore Sealing: An X-Ray Computed Tomography Analysis

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The shift from fossil fuel-based energy sources and toward more environmentally friendly, renewable alternatives highlights how important it is to properly plug and abandon oil and gas wells. Most depleted wells in the energy industry have been allocated for initial-phase abandonment, and cement has long been an appropriate material for permanently plugging these wellbores. Permanent plugging might not be appropriate everywhere, though, as depleted well sites provide a promising option for underground CO2 storage.

This work investigates the possibilities of short-term plugging solutions, with a particular emphasis on the application of novel thermal-sensitive polymer gels as an alternative sealing material. These gels provide a reversible and safe way to seal wellbores, keeping them intact for potential CO2 storage. The investigation of the polymer gel's flow through fractured chalk formations has been performed using X-ray computed tomography.

A wide range of experimental studies have been carried out in conjunction with real-time CT scanning to track the evolution of the polymer gel in chalk formations. The objective of this investigation is to ascertain the ideal concentration of the polymer gel and evaluate its efficacy in providing a temporary closure for the wellbores while ensuring their appropriateness for CO2 storage in the future. The research's conclusions have significant consequences for the oil and gas sector, especially when it comes to environmental sustainability and the shift to cleaner energy sources in the future.

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"Investigation of Growth-Relevant Parameters of Methanogens and their Impact on Hydraulic Properties and Substrate Conversion in Porous Media"

Authors: Andreas Loibner[1]; Elisabeth Edlinger[1]; Hannes Konegger[1]; Patrick Jasek[2]; Holger Ott[2]

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Microbial Impact on Subsurface Hydrogen Methanation:

"Investigation of Growth-Relevant Parameters of Methanogens and their Impact on Hydraulic Properties and Substrate Conversion in Porous Media"

The prediction of subsurface hydrogen methanation is crucial for large-scale hydrogen storage, thus enabling carbon dioxide utilization. To describe and model subsurface carbon dioxide reduction in the presence of hydrogen, a detailed understanding of substrate transport mechanisms and their impact on microbial growth in porous media is necessary. Accumulated microorganisms' impact on hydraulic properties, especially porosity and permeability, is central to access risks such as bioclogging. This study aims to address these complexities by performing microfluidic experiments under saturated flow conditions, using a realistic microbial consortium from a pilot site in Austria and Methanobacterium formicicum, a hydrogenotrophic model species the most abundant methanogen found in the reservoir brine.
The study specifically emphasized the impact of headspace gas composition (i.e., substrate gas concentrations), total pressure, nutrient availability, and the addition of organic substrates. The goal was to unravel the effects of these factors on microbial growth and methanation rates. Microfluidic experiments involved colonizing pore spaces with microorganisms and studying their growth and hydraulic properties. Biomass accumulation was characterized using high-resolution optical time-lapse images, and intrinsic biomass permeability was quantified through numerical pore-scale simulations. Despite biomass accumulation, a distinctive channel formation was observed, vastly retaining the original permeability. Matching simulation results to experimental pressure responses revealed a biomass permeability of approximately 100 ± 50 mD in all cases. These findings have significant implications:
(1) Clogging may be prevented by the observed channel formation, which allows nutrients to reach the biomass. (2) The high intrinsic biomass permeability may allow for an advective rather than diffusive nutrient supply, which may maintain high gas conversion rates. (3) Methanobacterium formicicum shows higher growth rates and a greater impact on permeability than the consortium, which explains the field observation and can be used as a design parameter for subsurface hydrogen conversion.
While preliminary results indicate disparities in conversion rates between the microbial consortium and isolated species, independent investigations in incubated core reactors align with the simulated methane yield on the field scale and analytically determined conversion rates during the microfluidic experiments.

Keywords:
Biofilm, microfluidics, reactive transport, biomass permeability, Archaea, Methanobacterium formicicum, geo-methanation, porosity-permeability relationship, hydrodynamics.

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884

Phase transition of salt mixtures in porous media during drying

using advanced optical microscopy, spectroscopy and X-ray tomography

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Abstract

Salt crystallization and dissolution induced by changes in air relative humidity stand out as a significant contributor to damage in construction materials [1, 2]. Aside from the visual impact on building structures, appearing as efflorescence, subflorescence may significantly influence the durability and structural integrity of materials as a result of stress-induced crystallization pressure [3]. Drying of building stones filled with salt-containing moisture is a common example of salt weathering [4]. Despite extensive studies on drying processes, precise forecasts of the evaporative drying rate and a comprehensive understanding of the various stages in drying remain major challenges, particularly when drying is coupled with salt deposition [5]. Effectively addressing the respective challenges requires a thorough understanding of the salt crystallization mechanisms within porous media [6]. In this study, we explored the response to humidity cycles in PDMS transparent micromodels and sedimentary porous rocks containing brine solutions of various compositions [7]. We specifically consider the case where air with different levels of humidity and at a constant temperature passes along one side of the porous media, leading to the formation of a drying front—a defined interface separating liquid-saturated and partially gas-filled domains. Digital optical microscopy, confocal Raman microscopy/spectroscopy, and 4D X-ray micro-computed tomography (μ-CT) [8] were used to visualize and characterize salt crystals in the porous media. We successfully detected the crystallization of the solution upon evaporation and the deliquescence of the crystal with increasing humidity. Systematic investigations were carried out to understand how the conditions for crystallization and deliquescence depend on pore space morphology and type of salt solutions. The results revealed the formation and growth of monocrystals as well as of opaque polycrystalline aggregates in the form of both efflorescence and subflorescence. The observed partial and complete pore blockage was restricted by throat and pore size and topology. The image data enabled us to accurately observe the interface between air, brine, crystal, and grain assisting in quantification of phase morphology. The findings highlight the potential of various visualization techniques for enhanced understanding of the transport-crystallization-dissolution coupling through in-situ experiments and hence for constructing more accurate prediction models and conservation strategies.

Keywords: Salt crystallization; Relative humidity; Evaporation; Micromodel; Confocal Raman spectroscopy; μ-CT; Porous media.

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MS16 / **885**

Membrane fouling and filtercake formation during static microfiltration harvesting of microalgae using thin glass fibre filters

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Micro-algae are being considered increasingly as an economic source for the sustainable production of biodiesel, food (additives), pharmaceuticals and nutraceuticals. However, the excessive cost and low efficiency of current microalgal harvesting processes limit the potential large-scale uptake of microalgal farming to transform industrial applications. Absence of universal separation methods, excessive energy inputs and hazardous chemical additives required are the main obstacles 1. In spite of these limitations, membrane filtration techniques dominate the harvesting of oil-rich microalgae 2. Filtration conditions have been adapted to optimize microalgal dewatering, including crossflow-, dynamic-, submerged membrane-, micro- and ultra-filtration. However, it has been suggested that static filtration may provide a simpler and more economical separation alternative, independent of cell motility, morphology, and surface charge. As a result, membrane filtration for the harvesting of microalgal cells has shown great promise and economic utility in recent studies. A challenging problem, however, in the filtration harvesting of algal suspensions is fouling of the membrane, leading to a continuous decrease of the filtrate flow rate. The foulants include suspended microalgal cells and their presumed Extracellular Polymeric Substances (EPS). To investigate this problem, we perform static microfiltration experiments, using thin glass fibre filters, to harvest oil-rich marine microalgae *Nannochloropsis oculata* [3]. Batch filtration experiments of microalgal suspensions using glass-fibre membranes are conducted under filtration pressures varying between 0.5 and 200 kPa. Here we investigate the relative importance of potential fouling mechanisms reported in the literature, including pore plugging, entrance blocking, and filter cake formation. 2 We examine variations in filtrate flux, using numerical differentiation of the filtrate volume to identify its scaling relationship with time and compare with the traditional root-time behaviour. These results are analysed

with reference to the blocking filtration laws to determine the potential fouling mechanism. Rheology tests of both filtration feeds and filtrate are performed, and both optical and scanning electron microscopy are used to observe the filtercake. Our results show a significant drop in the filtrate flux after a spurt loss phase under pressure. Scaling analysis demonstrates a power law relationship between cumulative filtrate volume and time in the post-spurt phase. We show here, for the first time, that the scaling exponent varies with time, approaching a value close to 0.5, i.e. root-time behaviour, only late after the initial spurt phase. Furthermore, our findings suggest that filtration of fresh microalgal suspensions experience a larger spurt loss compared to aged suspensions. This difference may be attributed to the limited production of EPS and microalgal debris during shorter cultivation periods. The microscopic observations reveal the invasion of microalgal cells into the porous membrane, which evidence the formation of an internal filtercake suggested by the blocking filtration laws. The invasion of microalgal cells results in significant membrane contamination, and the contamination rate increases with higher filtration pressures. Finally, we demonstrate that Fe3+ coagulant can be used to increase the microalgal particulate size before filtration, resulting in a much higher filtrate flux compared to uncoagulated suspensions. This result provides tremendous opportunities to reduce membrane contamination to a negligible level.

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Viscous Fingering in Miscible Systems: The Effects of Fluid Mobility and Velocity on the Mixing Zone Growth Rate

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Viscous fingering is an instability that occurs when a less viscous fluid displaces a more viscous fluid from a porous medium 1, 2, 3, 4. The viscous fingering instability results in small perturbations at the fluid-fluid interface (either a sharp, distinct, immiscible fluid-fluid interface or a fuzzy interface

between two miscible fluids), which progressively grow into distinct fluid fingers with time 1, 2. The instability can be triggered by differences in viscosity, fluid density and chemical reactions and hinders the operation and efficiency of various processes. For example, viscous fingering patterns can decrease the efficiency of oil recovery through water flooding 5, 6 and "dendritic growth"caused by viscous fingering leads to significant defects in crystals 7, 8. In chromatography, the viscosity of the solution being separated is dependent on the concentration and degree of adsorption of various components of the mixture. Visualization and tracer experiments have shown that preferential adsorption of the more viscous components leads to a viscously driven instability and deleterious mixing of the chemical fronts 9. Active and intentional control of interfacial instabilities is, therefore, an attractive area of investigation for many engineering applications 10, 11.

In this work, we investigate the interactions between viscous instabilities and the transport of miscible fluid species through diffusion and advection. Miscible rectilinear displacement experiments involving the displacement of glycerol solutions (20, 30, and 40 %) by water were conducted in a microfluidic chip with a homogeneous network of pores as shown in Figure 1 below.

In addition, we also investigate the impact of different fluid flowrates (0.5, 5 and 20 μL/hr) on the time-dependent evolution of the mixing front, changes in the concentration of the attenuating species (water), as well as variations in finger count, areal sweep efficiency and displacement kinetics. The finger count was seen to increase with increasing fluid viscosity contrast (M) as seen in Figure 1. Changing the fluid velocity did not have any significant effect on the finger count. Altering the fluid viscosity contrast also resulted in exponential changes in the kinetics of the displacement process, with fluid breakthrough occurring several orders of magnitude faster in advection-dominated displacement than in diffusion-dominated displacement. Our findings show that the concentration of the attenuating species in the mixing front is less than 30% for diffusion-dominated displacement and as high as 75% for advection-dominated miscible displacement (not shown in Figure 1). The mixing-zone width (ω) was found to be at least 7 times greater in diffusion-dominated displacement scenarios than in advection-dominated displacement scenarios.

Acknowledgements
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Multi-modal pore size distributions for low-density micro-porous carbons emerging from multi-modal virtual voids in quenched MD simulations

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The design of micro-porous carbons with desirable pore size distributions is of extreme importance for optimising the performance of battery and supercapacitor electrodes, as well as vehicular hydrogen storage. In the experimental synthesis of porous carbon materials, the porous characteristics can be controlled to some extent via varying pyrolysis temperature, chemical reagents, template size, and precursors. In many cases, however, it is very difficult to characterize the detailed microscopic structure of experimentally manufactured porous carbons. Atomistic simulation methods with reactive potentials have shown promise to fill this knowledge gap by creating realistic porous carbon structures. However, thus far such models have been unable to reproduce low-density microporous carbon structures due to clustering of atoms in high density regions, resulting in a small number of mesopores [Ranganathan et al.,2017]. Recently, we presented a new method using virtual voids, generating excluded volume by a soft repulsive potential which is progressively decoupled from the carbon atoms (Luo et al., 2021). This allows us to prevent densification and to create disordered carbon models with porosities up to 90%. We vary the size and density of the virtual voids and show that the mean of the pore size distribution and the accessible surface area can be controlled. By choosing the desired porosity and virtual void size, we create amorphous carbon models with mean pore sizes ranging from 10 to 32 Å, which agree favourably with experimental pore sizes for low-density microporous carbons. Our key findings were as follows: 1. Using virtual voids, the carbon atoms and pores can be distributed uniformly over the whole system to generate microporous carbon with an approximately Gaussian pore size distribution and porosity up to 90%. The addition of virtual voids produced no significant effects on the short-range bonding structure characteristics; 2. Using different sized virtual voids, we gain control over the pore size distribution and surface area of the final structure. A Gaussian function was fit to the pore size distributions, which worked particularly well for smaller virtual void radius. Almost entirely microporous structures, with pore sizes < 20 Å, could be obtained using a virtual void radius of 3-4 Å. At a density of 1 g/cc, mean pore sizes ranging from 10.3 Å to 21.6 Å were found using virtual void radii from 3 Å to 10 Å, respectively. Here we present our recent work generating multi-modal pore size distributions for low-density porous carbons, using multi-modal distributions of virtual voids. This allows us to make more accurate comparisons with experimentally generated micro-porous carbons, which often have a wide distribution of pore sizes. Indeed, by using a combination of up to three different virtual void diameters, see Fig.1, we

can create amorphous porous carbon structures with pore size distributions closely resembling experimental results. This enables us to create a comprehensive library of porous carbon structures using our multi-modal virtual void method, complementing the limited number of experimentally generated porous carbons. In turn, this enables the design of optimal carbon structures with respect to electrolyte permeability and carbon surface area.

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Pore-Scale Flow Properties of a high-porosity Carbon Fibre Graphite Felt Electrode for Redox Flow Battery Applications using large domain size micro-CT imaging and Lattice-Boltzmann flow calculations

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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 1 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 as a function of Representative Elementary Volume (REV) 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 computed using our home-grown Lattice-Boltzmann (LB) code (see [2,3]) on a big data set of 15 billion voxels using HPC facilities, in comparison with OpenPNM pore network calculations [4].

From this figure, we observe that the flow field 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. We carried out a detailed Representative Elementary Volume (REV) analysis, in terms of coefficients of variation of porosity and permeability as a function of increasing subsample size.
In addition, under certain electro-chemical conditions, H2 and O2 gas bubbles may develop in the pore space of the heterogeneous electrode, which has a detrimental effect on VRFB performance 1. Therefore we extend our multi-phase LB code to investigate the development of gas bubbles in the electrode (Fig.1b), initially by seeding random gas bubbles, based on our previous work on multi-phase flow in natural porous materials [5,6]. 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.

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MS01 / **890**

CO2 storage capacity in saline aquifers and uncertainty sensitivity analysis

Authors: Lishijia Han[1]; Yuan Zhang[1]

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Abstract: The emission of greenhouse gasses, especially carbon dioxide (CO2) is a major contributor to the global climate and the ecological environment. Geological storage of CO2 in deep saline aquifers is currently a widely recognized method with its stable storage and strong feasibility. However, researchers focus on the CO2 storage in saline aquifers, and there are few studies on the factors affecting the long-term stable storage of CO2 in brine. Therefore, the purpose of this study is to develop a long-term storage model and evaluate the performance of CO2 storage potential. First, we applied PC-SAFT (Perturbed-Chain Statistical Associated Fluid Theory) equation of state in phase equilibrium of CO2-H2O system. Results were validated against experimental data, indicating that PC-SAFT can well describe the phase behavior. Relevant property parameters of CO2-brine mixture were then modified and incorporated in the numerical simulation model. After that, the migration and distribution of CO2 stored in deep saline aquifers were simulated, examining the contribution of each mechanism over a 1000-year time scale. The correlations between reservoir temperature, residual gas saturation, horizontal permeability heterogeneity, the ratio of vertical to horizontal permeability, and pH were analyzed using Spearman's rank correlation coefficient method. Five storage efficiency indexes, including the Stratigraphic Trapping Index (STTI), Residual Trapping Index (RTI), Solubility Trapping Index (STI), Mineral Trapping Index (MTI), and Stable Trapping Efficiency (STE), were utilized as output parameters. The results indicate that different factors have varying degrees of influence on storage efficiency at different monitoring periods and mechanisms. Residual gas saturation is the main controlling factor for STTI, RTI, and STE at 100 years. At 500 years, the ratio of vertical permeability to horizontal permeability becomes the primary controlling factor for STI, and pH emerges as the dominant factor for MTI at the 1000-year mark.
This study provides a theoretical basis for evaluating CO2 storage potential in saline aquifers and selecting the optimal storage reservoir.
Keywords: Saline aquifers, CO2 sequestration, PC-SAFT, Storage capacity, Correlation analysis

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Poster / 891

Quantitative characterization method for residual oil distribution in heavy oil after multi-cycle steam huff and puff based on CT scanning

Authors: Haoyu Zheng[1]; Jian Hou[1]

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1. Objectives/Scope Steam huff and puff is an important development method for heavy oil reservoirs. An accurate description of the remaining oil distribution after steam huff and puff is crucial for guiding subsequent reservoir development. In this study, a new experimental apparatus was used to simulate the multiple cycles of steam huff and puff process more realistically. The occurrence state and distribution of remaining oil after different cycles of steam huff and puff were investigated.
2. Methods, Procedures, Process Laboratory experiments usually employ displacement to simulate steam huff and puff. In this study, a low-density and temperature-resistant material was used innovatively as the sand pack model, enabling multi-cycle steam huff and puff and in-situ CT scanning. The experimental procedures include steam injection, soaking, and recovery, with CT scanning of the sand pack model after each cycle. Based on characterization parameters such as shape factor and Euler number, the microscopic remaining oil is classified into network-like, cluster-like, film-like, and isolated droplet-like remaining oil. The proportions of these different types of remaining oil are compared after each cycle.
3. Results, Observations, Conclusion The viscosity of the heavy oil used in the experiment is 800 mPa·s (25℃). The statistical results indicate that as the number of cycles increases, the proportion of network-like remaining oil decreases, while the proportions of cluster-like, film-like, and isolated droplet-like remaining oil increase. From the first to the seventh cycle, the proportion of network-like remaining oil decreases by 34.11%, while the proportions of cluster-like, film-like, and isolated droplet-like remaining oil increase by 12.84%, 14.48%, and 6.76% respectively. The remaining oil transitions from a continuous distribution to a discontinuous distribution. This is because during steam injection, steam and heavy oil enter the intermediate container. During the soaking phase, steam is converted into hot water, forming an oil-water mixture with the oil. In the production phase, the oil-water mixture enters the sand pack, causing the network-like remaining oil to transform into cluster-like, film-like, and isolated droplet-like remaining oil, resulting in the discontinuous distribution of remaining oil. With an increase in the number of cycles, the water saturation increases, and the distribution of remaining oil becomes more dispersed.
4. Novel/Additive Information In this study, a new physical experimental model was developed to simulate the multi-cycle steam huff and puff process of heavy oil realistically. In-situ CT scanning technology was employed to quantitatively characterize the distribution of microscopic residual oil. This research guides the subsequent cold production of heavy oil.

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Poster / 893

Water Impact on Adsorbed Oil Detachment from Mineral Surfaces by Supercritical CO2

Author: Rui Gao[1]

Co-authors: Yulong Yang [2]; Wenyuan Sun [1]; Leilei Yang [1]; Jirui Hou [1]

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Geochemical reactions are crucial for in-situ CO2 mineralization underground associated with CO2-enhanced oil recovery (CO2-EOR) in a hydrocarbon reservoir. However, the presence of formation water and adsorbed oil on rocks generates physical barriers to CO2's access to mineral surfaces, which may yield impedance to CO2 mineral trapping that has yet to be accounted for. In this study, we mimic the dynamic oil detachment process using molecular dynamic (MD) simulations and analyzed the influence of an adsorbed oil film on supercritical CO2 (scCO2) diffusion towards the mineral surface in the presence and absence of a water phase. CO2-oil-water-rock reaction experiments are performed to substantiate the simulated data. Our results demonstrate a negative impact of water on oil film detachment by scCO2, which may give rise to a substantial delay in mineral reactions or even impede their occurrence and is unfavorable for mineralized CO2 storage underground. Carbonated water, regardless of whether it is saturated, showcases the same inhibitory effect on the miscibility of scCO2 and oil, thereby restraining oil film detachment and the contact of CO2 with the rock surface.

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Poster / 898

Molecular dynamics simulation of ionic diffusion and mixing phenomena in polymer-enhanced low-salinity waterflooding

Authors: Abdolmaleki Abdolmaleki[1]; Hassan Mahani[1]; Shahab Ayatollahi[1]; Nahid Pour Khiabani[1]

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Various studies have confirmed that water salinity and composition significantly impact the efficiency of the waterflooding process. Field-scale operation of low-salinity water injection has been

proven to be a cost-effective enhanced oil recovery (EOR) method as well as compatible with environmental regulations. The success of this technique relies on the contact of low-salinity water with the rock surface to alter the wettability of the rock to more water-wetting conditions. However, the salinity of the injected water increases, as it contacts the resident high-salinity reservoir brine which then significantly impairs the efficiency of this technique. Under flowing conditions, two main mechanisms affect the mixing phenomena: hydrodynamic dispersion and molecular diffusion. Our preceding laboratory research has clearly shown that if a small amount of polymer, such as HPAM (partially Hydrolyzed Polyacrylamide) is added to the injection low-salinity water it can significantly reduce the mixing zone by suppressing the diffusion and dispersion phenomena and increase the integrity of the fluid-fluid front. To gain a more in-depth understanding of this process, molecular dynamics simulations were performed to investigate the system at an atomic scale. Polymer molecules were introduced into the low-salinity water and the high-salinity and low-salinity waters were made laterally in contact, under no-flow conditions, to start mixing. Sensitivity analysis was performed on the main factors affecting this phenomenon such as the presence of polymer molecules, the effect of polymer concentration, the salinity of low salinity water, and the salinity of resident brine (i.e., the salinity difference). The results indicate that the time for full mixing is controlled primarily by the effective diffusion coefficient. By adding polymer, the polymer strands and their chemical interaction with the brine ions would act as a diffusion barrier and reduce the diffusivity of low-salinity water, enhance the viscosity, and delay the ionic diffusion phenomenon; thereby reducing the growth rate of the mixing zone. In all cases the mixing zone grew linearly with the square root of time; indicative of Fickian diffusive mixing. Once the diffusivity is reduced, the salinity profile becomes sharper, leading to a more effective low-salinity water effect, and less volume of injecting EOR agent is required at large scales.

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MS15 / 901

Machine learning algorithms for predicting breakthrough curves for pore scale reactive flow in porous media and application to parameter identification

Authors: Oleg Iliev[1]; Ivan Oseledets[2]; Daria Fokina[1]; Pavel Toktaliev[1]; Vasiliy Grigoriev[3]

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Reactive flows in porous media play an important role in our life and are crucial for many industrial, environmental and biomedical applications. Very often the concentration of the species at the inlet is known, and the so-called breakthrough curves, namely the time dependent concentration at the outlet, are the quantities which could be measured or computed numerically. The measurements and the simulations could be time-consuming and expensive, and machine learning and Big Data approaches can help to predict breakthrough curves at lower costs. Machine learning (ML) methods, such as Gaussian processes and fully-connected neural networks, and a tensor method, cross approximation, are well suited for predicting breakthrough curves.
In this presentation we discuss species transport with homogeneous or heterogeneous reactions for flow in porous media. The discussed ML methods are applicable for a broad class of single phase and multiphase, pore scale or Darcy scale reactive flows. Here we illustrate our developments in the case of pore scale single phase flow. The transport of species is modeled by a convection-diffusion equation, the flow is described by incompressible Stokes or Navier-Stokes equations. The surface kinetics is included via Robin boundary conditions in the case of heterogeneous reaction, or via source term in the case of homogeneous reaction. We present results on predicting breakthrough curves using the above approaches. Next, we discuss the application of the developed algorithms for deriving surrogate models to be used for solving parameter identification problems. We are interested in identifying the reaction coefficients, i.e. solving inverse problem. Solving inverse problem requires solving the direct problem many times (e.g. thousands). Replacing numerical solution of the problem by a machine learning model significantly speeds up the computational times. We use a number of numerical solutions to train the machine learning model and then use them to generate new curves, required to identify the parameters.

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902

Biological tissues as nanoporous materials

Authors: Natalya Kizilova[1]; Signe Kjelstrup[2]

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Biological materials are designed by nature as complex porous structures with sophisticated physical properties [1,2]. The porous composition serves as a supporting structure that supplies (i) mechanical strength and durability against external loads; (ii) long-range transport of fluids via specific networks of channels (blood and lymphatic vessels, lungs and gills, xylem and phloem veins, and many others); (iii) short-range diffusive transport; (iv) specific nano-scale transport with molecular motors, membrane channels, and others. The mass transfer phenomena at different scales of the tissues (from macro- to meso- and micro/nano scales) is a process that is connected with heat transfer. The latter is determined by metabolism and high body temperature in humans and the

warm-blooded animals, and the ambient temperature conditions for the cold-blooded animals and plants. The main feature of biological cells and tissues is a wide range of coupled physical processes as diffusion, chemical reactions with metabolic heat production, fluid flows, active contraction of molecular fibers, biological growth (a new mass production, pattern formation and morphogenesis), magnetic and electric properties. Therefore, thermodynamics of biological cells, extracellular structures and tissues must ground in the thermodycamics of small-scale systems (nanothermodynamics) [3].
In this work a comprehensive classification of porous structures of different plant and animal tissues is given. The common features and differences are analyzed. Coupled heat-mass-electric phenomena are observed. Some of the most important problems of transport in biology will be discussed with emphasis on how to obtain a macroscale description.

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MS03 / **903**

Non-Isothermal Variational Phase-Field Modeling in Hydraulic Fracturing

Author: xiaoqiang wang[1]

Co-author: Detang Lu [2]

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In this research, we present a novel numerical framework for hydraulic fracturing that incorporates thermo-hydro-mechanical coupled effects. Unlike previous studies that have employed the phase-field method for hydraulic fracturing modeling, our work introduces a THM coupling scheme grounded in the variational phase-field approach, a significant advancement in the field. The THM coupling is crucial for understanding underground fracture propagation, and our study extends the variational phase-field model to a thermoporoelastic medium. This integration enables the inclusion of fluid flow and heat transfer elements in fractured materials. We model fluid flow and heat transfer in the matrix and fracture independently and derive unified flow and heat transfer equations using phase-field calculus. To solve the THM coupled system, we develop an iterative solution algorithm

based on the fixed stress method. This algorithm effectively addresses the challenges associated with the coupled system. We discretize the proposed equations using the finite element method and employ a generalized Streamline Upwind Petrov Galerkin method for 8-node elements to mitigate numerical oscillations in advection-dominant issues within the heat transfer model. The accuracy of our model is validated by comparing the numerical results of fracture propagation with an analytical solution under the $\mathcal{K}$ regime. Additionally, we investigate the heat transfer process in a fractured domain, known as the Barends problem, using our model.

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904

The Effect of Cation Type, Salinity and Temperature on Hydrogen Diffusion into Brine: Implications for Underground Hydrogen Storage

Authors: Seyedeh Saba Kalati[1]; Shahab Ayatollahi[1]; Hassan Mahani[1]; Nahid Pour Khiabani[1]; Mohammad Amin Esmaeilbeig[2]

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The decrease in current fuel sources and their detrimental effects on the environment and climate have prompted a transition toward renewable energy sources. Since renewable energy sources are dependent on weather and seasonal changes, they could result in supply-demand imbalance. Hydrogen, as an energy carrier, can fulfill this energy gap. Storing hydrogen in underground formations, such as aquifers, has been the subject of extensive research recently. In these storage reservoirs, hydrogen can contact the resident brine and can be lost via the dissolution-diffusion mechanism. Therefore, successful designs of these storages require in-depth knowledge of hydrogen transport properties in reservoir brine. Experimental data on hydrogen diffusion coefficients in aqueous reservoir solutions are scarce. Additionally, there are significant discrepancies between the reported data, which makes it necessary to calculate reliable diffusion coefficient data. Molecular dynamic simulations have been applied in recent years to calculate hydrogen diffusivity in water. However, most of the available data relate to hydrogen diffusivity in pure water or NaCl-based solutions. Although NaCl is the dominant salt component in many aquifer waters, the presence of other salts could influence the hydrogen diffusivity as well. In this study, molecular dynamics simulations under realistic conditions of hydrogen storage reservoirs were conducted to calculate the hydrogen diffusion coefficient in various brines, containing monovalent (NaCl) and divalent salts (MgCl2 and CaCl2). The simulations were performed at various temperatures ranging from 323 to 373 K, a pressure of 200 bar, and salinities of 1 to 5 molal. The results show higher diffusivities at elevated temperatures and

lower diffusivities in more saline solutions. For instance, for a 1 molal solution of NaCl, the hydrogen diffusion coefficient was found 7.29×10-9 m2/s at 323K, increasing to 13.53×10-9 m2/s at 373K. This phenomenon is related to the higher kinetic energy of ions/molecules and the lower density and viscosity of solutions. The diffusivity is reduced by more than 38% at 353 K if the salinity rises from 1 to 5 molal. This diffusivity reduction is attributed to the presence of ions'hydration shells, which restrict the freedom of hydrogen molecules movement. Additionally, the hydrogen diffusion coefficient is smaller in solutions with divalent salts. This difference is more pronounced at elevated salinities. The results were analyzed in-depth to reveal the underlying mechanisms and provide new insight into the study of hydrogen loss in aquifers or water-saturated caprocks.

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MS13 / 905

Experimental study of gas flow and relative permeability in low-porosity media using LF-NMR

Authors: Aliya Mukhametdinova[1]; Desmond Batsa[1]; Timur Aminev[1]; Denis Bakulin[1]; Timur Unusov[1]; Alexey Cheremisin[1]

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The key characteristics of complex oil and gas reservoirs include high heterogeneity in the porous space, ultra-low permeability resulting from the nanoscale dimensions of pores, and the presence of solid insoluble organic compounds in the rock. These factors complicate the application of existing physical and mathematical flow models with sufficient accuracy. This causes challenges in accurately predicting producible hydrocarbon reserves and impedes the development of unconventional formations.

To enhance the characterization of the gas flow in low-porosity and low-permeability media, a detailed study of mass transfer is essential. This involves obtaining the relative permeability for multiphase systems that is typically determined from laboratory filtration experiments using rock samples. However, assumptions made during relative permeability determination, including methodological ones, often prove invalid when describing mass transfer in low-permeability porous media, resulting in quality of the field hydrodynamic model and increase development risks.

The objective of this study is to develop an enhanced laboratory-based method for determining gas-water and oil-water relative permeability in medium- and low-permeability reservoirs using NMR relaxometry under high-pressure conditions. NMR relaxometry enables the quick and accurate determination of sample saturation in tight rocks without additional contrasting during the core flooding experiment. The study considers surface phenomena in liquid-gas, liquid-solid, liquid-liquid, and gas-solid systems, determining their impact on mass transfer during filtration in rock samples. Experimental study was conducted using pressure-pulse decay porosimetry for obtaining reservoir

properties, low-field NMR relaxometry (2 MHz) on 1-inch core plugs and X-ray computed microtomography. Probes of degassed oil samples, deuterium oxide, carbon dioxide and methane were used as fluids in experimental modeling of the relative permeability.
As result, the method for determining the relative permeability in two-phase systems using NMR relaxometry was proposed. The current study also reports the results of fluid adsorption on crushed rock samples containing clays and organic matter using high-pressure NMR experiments. The analysis of results include the three-dimensional pore-network model based on experimental work. Validation of the model was conducted using values of reservoir properties (porosity, permeability, and pore size) determined by computed microtomography, as well as permeability values from the obtained relative permeability curves. In addition, sensitivity analysis of the developed pore-network model highlights the influence of pore connectivity, pore size distribution, gas phase diffusion on the absolute and relative gas permeability.

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MS15 / 906

A multi-well deep learning model considering geological and engineering parameters for the long-term forecasting of shale gas production

Authors: Yilun Dong[1]; Youzhi Hao[1]; Detang Lu[1]

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The production forecasting of shale gas wells is an important research topic in the natural gas industry. The underground pore structure is extremely complicated after hydraulic fracturing. Conventionally, researchers try to construct forecasting models via theoretical or experimental approaches. However, both theoretical and experimental approaches are faced with difficulties. Firstly, many parameters required during the theoretical computations cannot be timely or accurately measured, which limits the usage of theoretical models. Secondly, experiments can hardly match the real scale since a typical shale gas well has several thousand meters in length and depth. As a result, machine learning has become a popular modelling approach in the production forecasting of shale gas wells under complex pore structures induced by hydraulic fracturing.

With the large-scale development of shale gas blocks, an increasing number of production records as well as geological and well completion data is becoming available. This enables the construction of shale gas production forecasting models using dynamic time series data as well as static geological and well completion data. The former represents the historical production features of a well while the latter reflects the underground pore structure. Nevertheless, most existing methods do not incorporate static parameters into the modelling process. Moreover, most existing methods apply a

single-well modelling scheme where a model specifically trained for a target well is constructed. This scheme has two major flaws when it comes to field application. Firstly, it overlooks useful information from other existing wells in the same production block. Secondly, it requires a long piece of initial data for training and therefore cannot be used on newly developed wells. The problems faced with single-object methods have also been addressed in many other fields where the use of a long piece of initial data is impractical 1.

Considering the problems in existing shale gas production forecasting models, we propose a multi-well long-term forecasting model with static parameters. The proposed model is built on recurrent and fully connected neural networks and is trained on both production and static data from multiple existing wells. Since the training process does not need a long piece of production history from the target well, the proposed model can be used on a newly opened or re-opened well after a short initial period (for example, 14 days). Then, the long-term forecasting can be carried out iteratively using previously forecasted values. Therefore, the proposed model can achieve timely forecasting of shale gas production with both time-series data and pore structure after fracturing taken into consideration. The accuracy and usefulness of machine-learning-based shale gas production forecasting models are thus improved.

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Poster / 907

Production prediction of fractured horizontal wells in shale gas reservoirs based on multi-scale flow

Authors: Hongsha Xiao[1]; Man Chen[1]; Ruihan Zhang[2]; Yulong Zhao[2]; Zhongming Wu[2]

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[2] *Southwest Petroleum University*

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There are abundant shale gas resources in China. The technological recoverable resources amount to 21.8 trillion cubic meters, with a proven rate of only 4.8%, and the resource potential is huge. Shale reservoir permeability is very low. It must be fractured to obtain effective productivity. Moreover, the research on the special seepage law of shale gas reservoir is far behind the production practice: the complex multi-scale reservoir and flow space and various modes of existing of shale gas reservoir lead to strong non-linear and multi-transport mechanism characteristics of gas in the flow process,

and lack of comprehensive flow model to characterize the multi-scale flow law of shale gas reservoir; At the same time, complex fracture network is formed around horizontal wells. How to accurately simulate and predict the production performance after fracturing become the technical bottleneck of restricting the efficient development of shale gas reservoirs.
Considering the non-linear seepage mechanism of adsorption-desorption, slippage, Knudsen diffusion, surface diffusion, stress-sensitive effect, the mathematical models of shale gas seepage at different scales were established. The multi-scale seepage mechanism was coupled with the continuous medium-discrete fracture model, and the gas-water two-phase synthesis of multi-stage fractured horizontal wells in shale gas reservoirs were constructed. In order to avoid the large increase of mesh number and computation caused by local refinement around fractures by traditional orthogonal grids, based on unstructured triangular mesh and tetrahedral mesh, combined with the control volume-finite element (CVFE) method, a fully implicit numerical model of gas-water two-phase seepage was constructed. Finally, the effects of shale reservoir properties, multi-scale seepage, fracture network geometry and production system on the production performance of multi-stage fractured horizontal well and the optimization of parameters were studied.

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Poster / 910

Simulation study of hydrogen storage in a depleted gas reservoir: Microbiological influences in porous media

Author: Zanfu Xiong[1]

Co-authors: Jian Hou [1]; Qingjun Du [1]

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Storing hydrogen in depleted gas reservoirs is a viable method for balancing seasonal energy demand fluctuations. However, these reservoirs harbor a diverse population of microorganisms. H2 are considered one of the most important electron donors for subsurface microbial respiration. Under high salinity, high temperature, and high pressure conditions, microbial reactions such as methane generation, sulfate reduction, and acetate production are most common 1. These reactions result in hydrogen loss, gas acidification, pore plugging by metabolic biofilms, and alteration of the hydrogen-brine-rock three-phase interface properties due to the generation of organic acids 2. Currently, there is very little research on the impact of microorganisms in depleted gas reservoirs.
This study was conducted on a specific depleted gas reservoir, utilizing the CMG-STARS to simulate the impact of microorganisms on hydrogen storage. Firstly, the diffusive distribution of solid-phase microorganisms (biofilms) on porous media was designed, and Fick's law was employed to characterize the concentration-driven microbial transport process. Subsequently, based on reaction

conditions, four reactions were designed to generate CH4 (PH>7), H2S, acetic acid (PH<7), and microbial growth. The microbial population within the community was considered to control the rates of hydrogen uptake and microbial growth. The shedding of biofilms was influenced by the number of microorganisms and shear rate. Multiple sets of relative permeability curves were designed to match changes in wetting angle caused by acetic acid generation. Finally, the injection pressure was limited by reservoir fracture pressure and capillary forces causing leakage to the overlying formation. Seasonal hydrogen storage was conducted over four cycles, with a cycle consisting of 6 months of injection and 6 months of production.
The simulation results revealed the presence of high microbial saturation zones in near-wellbore region and higher parts of structure. The generated CH4 and H2S account for a maximum of 1.4% and 0.1% of the injected hydrogen volume, respectively, and accumulated below the H2 layer. The loss of hydrogen gas was highest at 5% in first cycle and decreased to a minimum of 0.6% in third cycle. As cycling period increased, the purity of hydrogen in produced gas became higher. Throughout the entire process, the effective porosity of the gas reservoir decreased by a value ranging from 0.1% to 0.5%, while the pH remained relatively unchanged.

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1. Thaysen, E. M., Armitage, T., slabon, L., Hassanpouryouzband, A., & Edlmann, K. (2023). Microbial risk assessment for underground hydrogen storage in porous rocks. *Fuel*, *352*, 128852. 2. Ali, M., Arif, M., Sedev, R., Sánchez-Román, M., Keshavarz, A., & Iglauer, S. (2023). Underground hydrogen storage: The microbiotic influence on rock wettability. *Journal of Energy Storage*,*72*,108405.

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Poster / 912

Pore-scale investigation of the influence of gas mixing on He/brine and CO2/brine wettability using Microfluidics: Implications for CO2 and H2 geo-storage

Authors: Amer Alanazi[None]; Hussein Hoteit[1]; Saleh Bawazer[2]

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Geological storage of hydrogen (H2) and carbon dioxide (CO2) is pivotal for a successful energy transition toward a diversified low-carbon economy and a net-zero emission future. The wettability

of reservoir rocks in the presence of formation fluids and H2 or CO2 is a controlling factor of gas mobility, residual trapping, and efficient storage. However, the influence of different brine types (salt type and concentration) and gas contamination on wettability is rarely reported in the literature.
Therefore, we present the results of a set of experiments using a microfluidic chip of different diameters (50, 70, 90, 110, and 130 μm) measuring CO2/brine, N2/brine, and He/brine advancing, receding, and static contact angles for the same brine type and mixing ratios (20%, 50%, and 80%) at constant conditions (P=14.7 atm and T= 22 ℃). The helium was used as an analogy for hydrogen to avoid any safety complications. The experiments were conducted using a constant brine rate at 0.1 μL/min during imbibition. A sophisticated Matlab code was built to measure contact angles from live videos of the microchips, allowing the generation of multiple data points with controlled upscaling.
The measurements indicate the channels are strongly water-wet for all gases with CO2 being the highest water-wet. All the dynamic contact angles decreased with increasing channel diameter from 50 to 130 μm. The measurements were validated with similar experimental approach in the literature. The CO2, N2, and He contact angles increased with increasing the mixing ratios from 10% to 50%. Higher hysteresis was observed with a higher mixing ratio, indicating a significant impact of contamination on the storage process.
The presented experimental approach depicts a time-effective technique to investigate crucial influencing parameters using microfluidic chips for effective and successful underground H2 and CO2 sequestration.

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MS09 / **913**

Volume of Fluid based study of the three phase dynamic contact line on rough surfaces relevant for Underground Hydrogen Storage

Author: Willemijn van Rooijen[1]

Co-authors: Hadi Hajibeygi [1]; Stephane Zaleski [2]

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Large-scale (TWh) renewable energy storage is crucial to achieve a net-zero green world. To accomplish this, renewable energy can be converted into hydrogen (H_2) and stored in large-scale volumes in giant subsurface geological reservoirs. The feasibility of underground hydrogen storage in porous

reservoirs highly depends on the flow and transport behaviour of hydrogen during subsequent injection and withdrawal cycles in the reservoir, which is governed by complex pore-scale processes [1-3].

Recently, several experimental studies [4-8] have taken place, which allow for the characterization of hydrogen transport properties in the subsurface. However, some discrepancies were found in contact angle characterization results using different measurement techniques and solid surfaces. The roughness of the solid surface is a possible explanation for this [9]. To date, no study has investigated the impact of roughness on the characterization of H_2-brine flow.

To help shed new light on the characterization of this crucial property, the Basilisk flow solver is used to conduct numerical simulations by solving the 2D two-phase Navier-Stokes equation. The H_2-brine interface is captured using the Volume-of-Fluid method, and the Continuous Surface Force method is employed to compute surface tension forces. The calculation of the curvature is done using height functions. To investigate the influence of surface roughness on H_2-brine flow in sandstone channels, a hybrid Volume-of-fluid coupled embedded boundary solver is used. Within this solver, an intrinsic contact angle can be imposed on solids with diverse shapes, facilitating the replication of a rough sandstone surface. Dynamic contact line motion and apparent contact angles can be analysed.

By comprehending the influence of surface roughness on the contact line motion, we will gain insight into the reported experimental measurements and assess the appropriateness of using specific data as input for larger-scale simulations.

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MS07 / **915**

Exploration of robust and fast L-splitting schemes for nonlinear double degenerate equations

Author: Ayesha Javed[1]

Co-authors: Koondanibha Mitra [2]; Iuliu Sorin Pop [1]

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Nonlinear advection diffusion equations model diverse physical phenomena.
Some examples include flow through porous media (as found in subsurface and reactive flows),biological processes, Stefan problem and permafrost models; and many others. In this work, we investigate numerical methods for nonlinear parabolic equations that show doubly degeneracy, i.e. for example the diffusion coefficient of the equation is allowed to vanish (degenerate diffusion) at zero concentration which leads to hyperbolic equation with free-boundaries as observed in nature, and become singular at full concentration leading to an elliptic problem. First we propose a semi-implicit (Backward Euler) time discretization. Implicit time stepping methods are popular due to their stability, allowing to avoid severe restrictions on the time step. This leads to nonlinear, time-discrete elliptic equations, for which linear iterative schemes are needed for approximating the solution, which combines the features of the Newton method and the L-scheme, i.e., a modified L-scheme. The linearization scheme is shown to be globally convergent (even for double degenerate cases). Moreover, it is linearly converging in the non-degenerate case accelerate with a small time-step. Numerical results will present which revealed that it is robust and stable when compared to the standard linearization schemes.

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Poster / **917**

Evaluation of the void space structure and flow channels in low-permeability reservoir rocks

Authors: Aliya Mukhametdinova[1]; Natalia Bogdanovich[2]; Alexander Burukhin[2]; Alexander Borisov[2]; Pavel Grishin[2]; Alexey Cheremisin[2]

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In recent years, the share of unconventional reserves in global oil production has been growing that leads to the development of efficient methods in exploration and development of tight reservoirs. The key features of low-porosity and low-permeability reservoirs are the high heterogeneity of the void space, the ultra-low rock permeability due to the nanoscale pores, and the presence of clays or solid insoluble organic compounds.

At the present stage of the experimental petrophysics, there is no standardized set of laboratory-based techniques for assessing the porosity, permeability and water saturation of such rocks. Thin layering, lenticularity, unpredictable changes in lithological characteristics (for example, heterogeneous clay distribution and carbonatization), reservoir properties and oil saturation of tight rocks create uncertainty in the petrophysical model, which, in turn, does not enable the accurate assessment of producible oil volumes.

Study of the composition (mineral, elemental and fractional) and structure of the void space can help to reduce this uncertainty in further modeling. The microstructure of the rock is determined by the geometry of the fluid flow channels, the size of these channels and their distribution. In other words, the characteristics of the reservoir properties of the tight rocks are always related to the parameters of the void space structure. Understanding of the void space structure can be obtained from theoretical calculations of various pore-pore connection models and from experimental works using direct and indirect laboratory methods. In this work, to examine and visualize the structure of the void space of low-permeability rocks, a set of modern techniques and equipment including gas porosimetry, computed microtomography (microCT), mercury porosimetry (MICP), nuclear magnetic resonance (NMR) and low-temperature adsorption / BET was used. Reservoir properties were determined for the rock collection of 45 core plugs and duplicate core samples. Additional tests include the X-ray diffraction analysis for determining the mineral composition and petrographic analysis of thin sections.

Results include the comparison of reservoir properties (porosity, permeability and pore size) determined by different techniques and discussion on advantages and limitations of each method for target low-permeability sandstone reservoir. The structure of the void space was characterized by pore size and pore throat distributions:the pore throats varies from 0.001 to 0.3 μm, the sizes of the pores ranged from 0.01 to 10 μm. The porosity of rock the collection varied from 6 to 14%, gas permeability did not exceed 0.2 mD. The contribution of the clay components and heavy hydrocarbons to the total porosity of samples in some intervals was demonstrated by results of NMR, microCT and MICP. Pore size distributions for the same samples by different methods were plotted jointly to illustrate the limitations of MICP, NMR thin section analysis and microCT at two resolutions. In conclusion, it is demonstrated how the reservoir properties and the void space (pores and pore throats) should be analyzed based on the results of both routine (gas porosimetry, liquid saturation, centrifuging, thin sections) and high-precision methods (NMR, microCT, low-temperature adsorption, etc.).

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MS06-A / 918

A three-layer Hele-Shaw problem driven by a sink

Authors: Meng Zhao[None]; Amlan Barua[1]; Shuwang Li[2]

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We investigate a sink-driven three-layer flow in a radial Hele-Shaw cell performing numerical simulations. The three fluids are of different viscosities with one fluid occupying an annulus-like domain, forming two interfaces with the other two fluids. Using a boundary integral method and a semi-implicit time stepping scheme, we alleviate the numerical stiffness in updating the interfaces and achieve spectral accuracy in space. The interaction between the two interfaces introduces novel dynamics leading to rich pattern formation phenomena, manifested by two typical events: either one of the two interfaces reaches the sink faster than the other (cusp-like morphology) or they touch each other (interface merging). In particular, the inner interface can be wrapped by the other to have both scenarios. We find that multiple parameters contribute to the dynamics including the width of annular region, the location of the sink, and the mobilities of the fluids.

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MS11 / 919

Microscopic Percolation Patterns in Multiphase Flow of CO2 Enhanced Oil Recovery and Mineralization

Authors: Qingxuan Wang[1]; Xiaopu Wang[1]

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

Corresponding Authors: wxp@upc.edu.cn, 3356877322@qq.com

The use of CO2 for secondary oil recovery has become a crucial means to achieve emission reduction. However, the microscopic transport mechanisms of water-oil-CO2 during this process, as well as the regulations governing CaCO3 precipitation in porous media leading to pore clogging and reduced permeability, remain unclear.

This experiment conducts a visualized study of CO2-oil-water percolation in homogeneous porous media, examining the impact of displacement factors such as flow rate and pressure on recovery. We quantify stable displacement, capillary fingering, viscous fingering, and other modes. Based on CO2-oil-water percolation experiments, a buffer solution is injected under different flow rates and pressure conditions to catalyze and accelerate CO2 mineralization reactions. The experiment

observes the microscopic aggregation and distribution patterns of CO2 mineralization crystals in porous media, exploring the resulting changes in pore volume and their corresponding effects on permeability and fluid mobility.

This experiment employs a specialized pressure-resistant microfluidic chip with a CaCO3 coating, accurately simulating the geometric structure and surface properties of underground rocks. The chip initially exhibits an oil-wet surface, and upon injection of low-concentration desalinated seawater (referred to as desalination water), cations in the desalination water transform the wettability of the rock crystals, causing certain coatings to transition to water-wet characteristics. Before the breakthrough of desalination water, there is a positive correlation between the internal pressure of the chip and the injection flow rate, while it exhibits a negative correlation with pore size. The heterogeneity of pore shapes and sizes in heterogeneous media results in higher injection pressure compared to homogeneous media. After the injection of supercritical CO2 (ScCO2) into the chip, the remaining water dissolves some CO2, creating an acidic environment within the chip, and corroding the CaCO3 coating within the channels. However, the chip also contains ScCO2-encapsulated media, preventing corrosion and forming a protective phase. ScCO2 can similarly alter the crystal wettability, transforming it into CO2-wet. Injection of a buffering solution to adjust the internal environment of the chip to alkaline conditions results in the formation of CaCO3 crystals adsorbed on the surface of the porous media. Nevertheless, Some crystals tend to aggregate, indicating that CaCO3 might bridge at the pore entrance, potentially causing blockages.

This study focuses on the fundamental mechanism analysis of CO2 multiphase flow and sequestration, researching improvement measures for CO2 enhanced oil recovery and storage technologies. It lays a crucial research foundation for enhancing petroleum recovery, contributing to the achievement of carbon peaking and carbon neutrality goals.

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MS13 / 921

Effect of partial saturation on acoustic properties of nano-porous media

Author: Gennady Gor[1]

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Nanoporous materials provide high surface area per unit mass and are capable of fluids adsorption. While the measurements of overall amount of fluid adsorbed by a nanoporous sample are straightforward, probing the spatial distribution of fluids is non-trivial. For macro-porous media the effect of partial saturation on acoustic properties is described by the theory of poroelasticity.

To test applicability of poroelastic patchy saturation models to nano-porous materials, we consider ultrasonic measurements during adsorption and desorption of n-Hexane vapor on nanoporous Vycor glass (Page et al., 1995). As vapor pressure is increased from zero to the saturation pressure, the vapor is adsorbed on the pore walls, resulting in gradual increase of the liquid fraction. The reverse process occurs when pressure is decreased, but the 'drying' of the nanopoorus glass is heterogeneous, resulting in a very different velocity-saturation relationship.

On adsorption, we model ultrasonic properties of partially saturated glass using Continuous Random Model (CRM) of Müller and Gurevich (2005), also known as the Dynamic equivalent medium approach (DEMA). In this model, the liquid fraction is considered a random function of position, controlled by the correlation length d ("patch size'), which may itself vary with saturation.

As noted by Kobayashi and Mavko (2016), during imbibition, some significant portion of the liquid fraction should be uniform. In other words, if we consider the medium to be saturated with a binary mixture of two fluids, one of these fluids should be liquid, while the other should be a uniform mixture of liquid and vapor with liquid fraction SL0, which itself increases with the increasing overall liquid saturation SL. This is even more so for nanoporous media, where adsorption tends to produce rather uniform patterns. Our modelling shows that there is a strong coupling between the patch size and uniformly saturated fractions, which cannot be resolved with ultrasonic data only. However, this can be resolved using light scattering data (Ogawa and Nakamura, 2013). Very weak light scattering during adsorption shows that 99.3% of the increase of the saturation is uniform. Yet the saturation is not entirely uniform, as shown by the deviation of the longitudinal modulus from the unform saturation limit (as discussed in the next section).

The desorption process results in macroscopic liquid patches, and cannot be modelled with CRM. We model this process with elastic finite element methods.

Our calculations show that on adsorption the characteristic patch size is of the order of 100 pore diameters, while on desorption the patch size is comparable to the sample size. These results are supported by optical data for similar systems. Our analysis suggests that one can employ ultrasound to probe the uniformity of fluid spatial distribution in nanoporous materials.

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MS17 / 922

A vectorial finite element method for the pore-scale calculation of the high temperature thermal behaviour of periodic porous 3D architectures.

Author: Benoit Rousseau[None]

Co-authors: Franck Enguehard ; Jérôme Vicente ; Yann Favennec

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In the field of carbon-free heat power generation, there is a growing interest in the design of compact and long-life high-temperature energy systems (HTES), such as thermochemical reactors, volumetric solar receivers and radiant tube inserts, among others. These energy converters have long been based mainly on porous reticulated ceramics (porosity ~75-95%, cell size ~0.1-10 mm) which can be described as a continuous ligament network delimiting open cells through which a heat transfer fluid (reactive or not) can flow. The rapid development of processes based on the principle of additive manufacturing (AM) has recently extended the possibilities of fabricating new 3D periodised geometries ranging from hierarchical structures with different sets of unit cells to triply periodic structures with minimal surfaces. From a thermal modelling perspective, one of the main challenges is to accurately account for the exact contribution of thermal radiation from these new geometries in the HTES heat balance, both in transient and steady state. To tackle this challenge, two main numerical modelling approaches can be used today to determine the temperature and/or heat flux fields within the 3D structures. The first class of approach, at the continuous macroscopic scale, requires the radiative transfer equation to be solved rigorously as long as the ceramics studied follow a radiative behaviour governed by the Bouguer-Beer-Lambert law, i.e. the extinction of thermal radiation is characterised by a negative exponential function of the optical thickness. This integro-differential equation can then be simplified into an equivalent - but approximate - thermal conduction equation by respecting the appropriate Rosseland conductivity assumption if the medium is optically thick. When the optical thickness becomes smaller (<3), other more advanced analytical and numerical approaches can be used: P1 approximation, discrete ordinate method, Monte Carlo method. However, the recent regular 3D architectures obtained by AM processes clearly show, unlike the more conventional open-cell foams, a radiative behaviour that clearly deviates from the well-known beerian behaviour, which leads to the thermal problem being solved by calculations carried out at pore scale. The concept is to treat elementary heat exchanges at the pore scale using a representative 3D image of the ceramic, beforehand obtained by X-ray μ-tomography or by computer-aid based generation. Using a scheme implemented in a solver based on vectorial finite elements, we here propose a 3-step method for cases where convective transport is neglected: (i) solving the heat equation in the solid skeleton (ii) solving the radiative transport in the fluid phase (iii) solving the conductive-radiative coupling at the fluid-solid interface. This presentation will show the results of temperature fields calculated in periodised structures and will allow us to discuss how to model radiative transport on a continuous scale when beerianity is not satisfied.

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MS01 / **923**

Evaluating the Material, Energy, Environmental, and Economic Aspects of Pan-European CCS Infrastructure

Author: Ali Eftekhari[1]

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Carbon capture and storage (CCS) holds immense promise for mitigating climate change, but its full potential remains largely untapped due to challenges in sourcing CO2 and constructing an extensive infrastructure across Europe. To address these limitations, we present a workflow and an open-source Python package that assesses the material, energy, environmental, financial, and operational aspects of pan-European CCS networks. Our tool leverages a spatial map of European emitters based on the E-PRTR database, incorporating flue gas composition information to tailor capture techniques to each emitter's industrial sector and proximity to existing or potential pipelines and storage sites.

Our computational model employs a Graph data structure to construct a network that connects emitters along existing European gas pipelines and power cables, simulating potential future pipeline routes. Multiple transportation routes, represented as Directed Graphs, link emitters to subsurface storage sites in the North Sea. The tool performs detailed sizing calculations for pipelines, designs compressor and pumping stations and temporary storage tanks, and calculates compression energy and cost for subsurface storage. Energy consumption is determined based on process models, and correlations are applied for capital cost estimation. Operating costs are projected using the spatial cost of fuel and electricity across Europe. A multistep approach to database analysis and design and energy analysis steps ensures the computational efficiency of the package for sensitivity analyses and case studies for minimizing cost and energy demand.

Preliminary results from our model indicate that a German-Danish CCS network, with storage in depleted Danish North Sea reservoirs, will demand electricity and heat equivalent to two- and one-fold Danish consumption, respectively. This network, connecting emitters with annual emissions exceeding 50,000 tons, is projected to store approximately 350 Mt of CO2 annually. However, due to the carbon intensity of the grid and heat, this network will also emit an equivalent of 30% of the stored CO2. A substantial capital investment exceeding EUR 90 billion, primarily allocated to pipeline construction, is anticipated. An annual operating cost ranging from EUR 6 to 18 billion, depending on electricity prices, is also projected.

Our software is distinguished by its utilization of updated emitter databases, fundamental process models, and state-of-the-art efficiency factors and costs provided as process equipment databases. These features minimize user input and ensure realistic network design and accurate estimations of environmental footprints, energy demand, capital, and operating costs, facilitating informed planning and decision-making by taxpayers, investors, operators, and policymakers.

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924

Lattice Boltzmann Method for Multiphase Flow with Phase Change

Authors: Guang Yang[1]; Moran Wang[1]

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Corresponding Authors: 13121958175@163.com, mrwang@tsinghua.edu.cn

Multiphase flow with phase change is ubiquitous in many industrial applications including Enhance Oil Recovery(EOR) , Carbon Capture Storage(CCS) and fuel cell. In this work, we present a lattice Boltzmann model(LBM) for multiphase flow with phase change. Coupling color-gradient model and pseudo-potential model, current model is capable of capturing phase change in porous media spontaneously as well as immiscible multiphase flows. A new correction term is introduced into the color-gradient LBM. The proposed model is comprehensively verified via multiple benchmarks. Pore-scale simulations are conducted after benchmarks. Our results indicates the significance of considering phase change in pore-scale studies.

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MS07 / **925**

Fully coupled implicit discretization for large-scale simulation of miscible multiphase flow in heterogenous porous media

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To comprehensively understand and predict the behavior of CO2 storage, the development of precise mathematical models and advanced numerical schemes for large-scale simulations is demanding. The advection and diffusion or even interaction between injected supercritical CO2 and other fluids in the storage reservoirs should be able to be described by multiphase flow models. Notably, the consideration of CO2 dissolution introduces dynamic changes in the density of fluid phases, instigating density-driven flows. Most discretization schemes are explicit or semi-implicit which restricts the time step size of the simulations. In this work, a fully coupled and fully implicit scheme for large-scale simulations of miscible multiphase flow in heterogeneous porous media is proposed. Vertex Centered Finite Volume Method is employed for the spatial discretization. The linearly implicit extrapolation method (LIMEX) is adapted for temporal discretization. The arising linear system of

equations is solved by BiCGSTAB with Geometric Multigrid (GMG) preconditioner. The parallel implementations are based on the open-source software: UG4. The validation of the proposed scheme is verified by the comparisons with analytical solutions in benchmark cases. The weak and strong scaling tests are performed on the supercomputer Shaheen II with up to 4096 processor cores. Due to the stable numerical treatment and efficient implementation, the proposed scalable solution is suitable for large-scale simulation over long periods.

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Poster / 926

Multiphase Flow Through Rough Porous Layers in Proton-Exchange Membrane Fuel Cells (PEMFCs)

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Polymer electrolyte membrane fuel cells (PEMFCs) have emerged as ideal energy-conversion devices for hydrogen energy applications. The performance of PEMFCs is significantly affected by the accumulation and transport of water inside porous components and flow channels. Here, we focus on investigating the role of surface roughness on the fluid transport and droplet impact behaviours in the porous components of PEMFC. We start by examining the fluid transport characteristics at the interfacial region of microporous layer (MPL) and catalyst layer (CL), considering the effects of compression stress, porosity, and wettability. Liquid and gas permeabilities are also investigated to assess water drainage and fuel supply efficiency with different compression conditions. Then, surface roughness effects of gas diffusion layer (GDL) on liquid droplet removal inside a flow channel are investigated. We simulated the complete process of droplet removal in flow channel, including emergence, growth, detachment, and removal. We also identified different regimes of detachment modes based on the droplet breakup location and detachment ratio. Finally, we experimentally examined the liquid droplet impact dynamics on rough surfaces with various topological parameters. We observed different modes of droplet spreading and bouncing behaviour, and droplet impact outcome transition from bouncing to no bouncing is identified. To quantify the influence of surface wetting area on the bouncing-wetting transition, we proposed a modified Weber number that incorporates a combined effect of droplet kinetic energy, surface energy, and adhesion force. We found that the droplet impact outcomes in the transition regime can be accurately described by a single curve as a function of the modified Weber number. The results can provide valuable insights into selecting appropriate parameters of diffusion media for optimising water management and fuel supply during fuel cell operation processes.

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928

Understanding the Role of Wettability Distribution in Underground Hydrogen Storage (UHS) in Heterogeneous Aquifers

Authors: Mansour Nazari[1]; Matin Bagheri[1]; Hassan Mahani[1]; Shahab Ayatollahi[1]

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Hydrogen is recognized as a clean energy carrier and plays a key role in energy transition. Subsurface structures, such as aquifers with enormous storage capacity and global abundance, are economically viable and highly promising for hydrogen storage. However, the formation rocks of such structures bear various complexities, including different minerals contributing to the rock structure, as well as complex pore structures such as microporosity, microfractures, etc. Therefore, understanding the flow dynamics of hydrogen and water in these formations is essential to optimize hydrogen storability and recovery. The goal of this paper is to investigate the effect of flow regime and wettability distribution on flow pattern, trapping mechanisms, and hydrogen recovery efficiency through direct computational fluid dynamics simulations. To do so, by applying direct numerical simulation (DNS) and finite volume techniques, the governing flow equations were directly solved in realistic pore-scale geometries while considering various types of wettability distribution in the porous medium. The results reveal that moving toward a less water-wetting state during the primary drainage (or storage) process reduces hydrogen trapping, allowing for more pore space to be available for hydrogen storage. This is because hydrogen faces less capillary resistance and gains higher effective permeability. However, during the imbibition (or recovery) process, it slightly increases hydrogen trapping in relatively large pores due to the larger capillary pressure in pore throats, which reduces the efficiency of hydrogen withdrawal. Therefore, changing the wettability of the storage system to a less water-wetting state favors the initial distribution of hydrogen for underground hydrogen storage operation. This modification reduces residual hydrogen saturation, increasing the ultimate hydrogen recovery factor. This paper also presents and discusses further simulation results on the effect of initial wettability distribution on the UHS process.

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Prediction of Permeability of Multi-Scale Anisotropic Porous Media by a Novel Software Suite PoroS

Author: Elena Syerko[1]

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In porous media science and engineering permeability is one of the key properties, which defines the capacity of porous structure to be penetrated by a fluid. Fibrous materials used as reinforcements of structural composites can be considered as the most general and complex class of porous media due to their anisotropic and multi-scale character: an engineering textile is composed of yarns at meso-scale, themselves composed of thousands of fibers at micro-scale. Experimental determination of permeability of fibrous textiles is a tedious task. It is time-consuming, requires a specialized and often costly equipment, and almost impossible to be conducted at micro-scale. Virtual characterization of permeability using numerical methods has important advantages over the measurements. It allows to reduce material waste, to analyze the influence on permeability of material microstructural parameters, while being capable of addressing high variability inherent to this class of materials. At present there is no widely accepted numerical approach for permeability prediction yet due to modeling challenges such as the choice of the RVE (representative volume element), boundary conditions, permeability identification technique, as revealed in the first international virtual permeability benchmark on fibrous media 1. This motivated the development of a novel scientific software named 'PoroS' 2, which includes a set of numerical solvers specifically designed for anisotropic multi-scale materials for the prediction of permeability.

This scientific software can calculate the saturated permeability of a porous material based on real 3D images of its micro/mesostructure. Alternatively, digital twins of the material can also be used as input to PoroS.

The first version of the software PoroS 1.0 has been developed to compute the permeability of materials with single-scale porosity. The Stokes flow problem is solved using the finite element method and specifically designed matrix-free iterative solvers to reduce the computational cost. The pseudo-compressibility formulation is employed, and the full-field homogenization method [3] then allows the full 3D permeability tensor to be calculated using only the computed velocity fields, giving the advantage of reducing the number of degrees of freedom without having to compute the pressure field.

After having validated the flow solvers using a set of test-cases from the literature, PoroS predictions were compared with the results of the first stage of the virtual permeability benchmark 1. The input geometry was a 3D image with a nominal resolution of 0.5 μm/voxel representing the microstructure of a yarn composed of ~400 slightly misaligned fibers (available on the repository at https://doi.org/10.5281/zenodo.6611926). The results obtained using PoroS 1.0 fell within the main cluster of results of the benchmark (Figure 1) and are close to the mean value defined after elimination of outliers.

The second version of the software PoroS 2.0 [4] addresses the permeability of materials with dual-scale porosity by using the Stokes-Brinkman flow problem formulation. PoroS 2.0 is officially involved in the second stage of the virtual permeability benchmark [5] dedicated to permeability of the material at the mesoscopic scale of the textile, in particular, a textile for which experimental measurements were available. The comparative analysis of results is ongoing.

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Poster / 930

Reshaping the Imaging Landscape: AI-Supercharged Swin Transformer for Unprecedented Detail

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Super-resolution imaging, a transformative technique spanning various scientific disciplines, holds the potential to revolutionize our understanding of complex porous structures within the realm of porous media and modeling. Traditional imaging approaches often struggle to capture the intricate details of porous media's intricate structures. To overcome this limitation, our research employs advanced AI-driven super-resolution methods, aiming to transcend inherent resolution constraints. Our goal is to bridge the gap between large-scale imaging methods, which excel at capturing macroscopic features, and small-scale techniques known for their detailed focus. By developing techniques to reconstruct high-resolution representations from lower-resolution inputs, our study promises a profound characterization of porous media's internal architecture, critical for applications such as filtration, oil recovery, and groundwater flow.

Our research journey embarked with a meticulous exploration of AI-based super-resolution techniques. Initially, we employed the ESRGAN model with the rrdb net as the generator. While it exhibited commendable performance, the model's large size posed practical challenges. Subsequently, we transitioned to the SwinIR model, which delivered results characterized by their remarkable smoothness and sharpness. Building on this progress, we leveraged GAN-assisted Swin transformers, an approach that not only yielded exceptional outcomes but also presented a significantly reduced model size. This transition not only streamlined GPU memory usage during training but also accelerated the training process.

Our methodology included in-depth examinations of various loss functions, highlighting the significance of a hybrid approach that combines GAN loss and pixel loss. This novel approach proved instrumental in effectively training the model and enhancing the quality of super-resolution results. Throughout our research, we meticulously studied the individual impact of each loss function and established relevant metrics, providing a robust foundation for our study's methodology.

Beyond the advancements in super-resolution techniques, our research culminated in the development of a model capable of achieving super-resolution beyond current technological limitations. This breakthrough allowed us to push the boundaries of resolution in porous media imaging, and we validated our findings on new datasets with resolutions of 1μm, 4μm, and 16μm.

The results were nothing short of groundbreaking. We observed that our AI-driven super-resolution approach consistently outperformed conventional methods, producing images with unprecedented clarity and detail. Notably, our model achieved remarkable results even at resolutions previously considered unattainable. This newfound capability opens doors to a wealth of possibilities in the fields of porous media analysis, offering insights that were once hidden from view.

In conclusion, our research demonstrates the immense potential of AI-driven super-resolution in revolutionizing porous media imaging. By unveiling hidden details and pushing the boundaries of resolution, our findings hold promise for a wide range of applications, from enhancing filtration processes to optimizing oil recovery and improving our understanding of groundwater flow dynamics.

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Poster / 931

The implications of subsurface CO2 geological storage for mineralogy and geomechanical behavior: Triassic Sherwood Sandstone, East Irish Sea, UK

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There is a growing recognition of the need to reduce the atmospheric concentration of Carbon Dioxide (CO2) to slow the effects of climate change. Many sedimentary basins, which host prolific hydrocarbon resources, are now being reassessed for their potential role as subsurface storage sites, including the East Irish Sea, UK. However, there are implications for subsurface CO2 geological storage, such as mineralogical alterations due to the acidic character of pore fluids and potential changes in pore space and grain character. Such rock-fluid interactions may have consequences for the geomechanical behavior and petrophysical parameters.
In this study, we undertake an integrated method through hydrothermal and mechanical experiments to assess the impacts of CO2 storage by comparing the pre- and post-reacted samples in terms of mineralogy, petrophysical parameters and geomechanical behavior of Triassic sandstone core from the Sherwood Sandstone Group, South Morecambe Field, (110/8a-C5) East Irish Sea, UK. The Triassic Core samples are subarkosic arenites made up mainly of quartz, K-feldspar, dolomite and illite which are determined using optical microscopy, SEM and XRD. Detailed SEM images and SEM-EDX mapping illustrate dolomite cement, partial alteration of K-feldspars and illite coating the quartz grains, which was largely responsible for porosity preservation. The density and porosity of the pre-reacted samples are 2.1g/cc and ~15 - 20.5% respectively. The confined permeability is 1.9e-19m2. In terms of the rock's geomechanical behavior, the Young's Modulus obtained after the triaxial loading test is 5.3GPa. Hydrothermal reactor experiments were carried out in a cylindrical stainless steel Parker Autoclave Engineers with 500 ml volume, the vessel was heated by a ceramic band heater at 80℃ and the pressure was raised and kept constant at 20 MPa. In each experiment, the vessel was partially filled with a seawater-like fluid, the Triassic sandstone core was immersed in this fluid, CO2 was injected into the remaining space and the autoclave was pressurized. The remaining fluid was analysed for key chemical species using ICP-OES to help the understand mineralogical alterations and potential authigenesis.
Carbonate dissolution, increase of the alteration degree of K-feldspar, subordinate Illite precipitation or even dissolution in the hydrothermal reacted sample can be expected leading to the modification of pore space and rock cohesion. Considering that mineral dissolution is the main rock alteration process, an increase in porosity and permeability can be expected. Conversely, the density and Young's Modulus can have smaller values mainly due to the loss of dolomite cement and consequent rock weakening.
Investigating the potential physical changes in porosity, permeability and rock strength and comparison of the results from pre- and post-experiments, is crucial to assess which are the main reactive minerals and classify the best and safest rock facies for a subsurface CO2 geological storage. The results presented will be used to predict the best petrophysical facies and improve our understanding of injecting CO2 to avoid fractures and fault reactivation.

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Poster / 932

Comparisons between a dual-pore-network model and a hybrid pore-network-continuum model for predicting permeability and formation factor of multiscale carbonate digital rocks

Authors: Bowen Shi[1]; Chao-Zhong Qin[1]; Xingyuan Zhao[1]

[1] *chongqing university*

Many underground rocks have been found to possess complex multiscale porous structures with bimodal/multimodal pore size distributions, such as carbonate rocks, tight sandstones, and shales (Bultreys et al., 2016; Shan Wang et al., 2022; Nijat Hakimov et al., 2022). Flow and transport in these rocks play an important role in many subsurface applications. In addition to in-situ core experiments, several pore-scale numerical models have been developed to simulate flow and transport in multiscale porous structures, including dual-pore-network, micro-continuum and pore-network-continuum models (Francisco J. Carrillo et al., 2020; Zhang et al., 2021; Tom Bultreys et al., 2015). Compared to micro-continuum and pore-network-continuum models, a dual-pore-network model is computationally efficient and can be used to the full core analysis. However, the effect of smearing heterogeneity of microporous domains (i.e., sub-resolution domains) on numerical predictions needs to be studied.
In this work, absolute permeability and formation factor of Estaillades carbonate rocks are modelled by both a dual-pore-network model and a hybrid pore-network-continuum model. We show the key difference between the dual-pore-network model and pore-network-continuum model for treating microporous domains. By comparing numerical predictions of the two models, the influence of microporous heterogeneity on seepage characteristics of carbonate rocks is extensively explored. Moreover, the dual-pore-network model is used to study the influence of image resolution on the prediction of permeability and formation factor. As reducing the resolution of the original image, it is observed that more and more resolved pores are identified as microporosity, while the modelled permeability decreases.

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Evaluation of the Mechanisms and Performance of Ionic Liquids in Shale Swelling Inhibition at 250 oC using Molecular Dynamics and Experimental Analysis

Authors: Banet AJuna[1]; Xuan Li[2]; Lixin Zhu[2]; Wuzhen Gong[2]; Ruiyu Bai[2]; Weian Huang[2]

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1.0 Introduction

Over 50 % of reservoirs worldwide contain water-sensitive shale formations containing exorbitant compositions of clay minerals 1. Over 70 % of shale is composed of smectite (montmorillonite) resulting in over 90 % of the wellbore instabilities in the drilling worldwide2,[3]. Gautam et al. [4] also reported that mud systems are significantly destabilized while drilling deep and ultra-deep shale reservoirs with bottom hole temperatures (BHTs) above 200 oC due to the disintegration of their additives.

Due to the toxicity of oil-based drilling fluids, water-based drilling fluids (WBDFs) are being used for drilling activities because they are non-toxic, cheaper, and easier to prepare and use2,[4]. However, when water molecules from WBDFs come into contact with shale formation, they interact with clay minerals leading to the swelling of the formation[5]. This results in the leakage of mud into highly porous and poorly consolidated formations, the collapse of the wellbore, reduction in the rate of drilling by the bit, abnormal viscosity of mud, bit balling, sticking, and reduction in the permeability of the reservoir 2,[6].

The physicochemical properties of "green"and "designer"ionic liquids (ILs) such as compatibility with different compounds, favorable solvating potential, excellent thermal stability, high ionic conductivity, high solubility, and higher surface activity have made them excellent potential additives for preventing swelling of clay minerals under high pressure and high temperature (HPHT) conditions [7],[8]. This is because conventional inhibitors for example polymers, surfactants, and ionic salts decompose at higher temperatures which negatively affect their performance in preventing the swelling of shale[9],[10]. Therefore, more research is required to establish the type of ILs that has optimal performance at HPHT conditions.

2.0 Methods

Rheological and filtration properties at 250 oC and shale cuttings recovery experiments at 250 oC, linear swelling experiments, were utilized to establish the performance of imidazolium, ammonium, and pyrrolidinium-based ILs in a 4 wt% sodium montmorillonite (Na-Mt) dispersion. Mechanisms for shale swelling inhibition were established by X-ray diffraction analysis, zeta potential tests, particle size distribution, contact angle measurements, and molecular dynamics simulations with Material Studio software version 2019.

3.0 Results

The addition of ILs in the Na-Mt dispersion at 250 oC was associated with an improvement in the rheological properties, better filtration properties, an increment in the percentage of shale cuttings recovered, a reduction in the rate of swelling, higher values of contact angle, and a reduction in the d-spacing between the sheets in Na-Mt due to strong electrostatic and van der Waals forces of attraction between the cationic group and the surface, interlayers, and edges of Na-Mt sheets. Their performances at HPHT conditions are strongly controlled by the nature of the cationic group with imidazolium > Ammonium > pyrrolidinium cations due to varying strengths and polarity of bonds formed during adsorption onto the active sites of Na-Mt.

4.0 Conclusions

Imidazolium-based ILs reported the best shale inhibition performance at temperatures above 250 oC. They are the most stable ILs at temperatures above 250 oC.

Keywords: shale swelling inhibition, water-based drilling fluid, Ionic fluid, High temperature and high-pressure conditions.

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The role of bio-geotechnics in reducing greenhouse gas emissions from constructional slope stabilization

Authors: Farshad Yazdani[1]; Pouya Alipanahi[1]; Hamed Sadeghi[1]

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In the last few decades, the concepts of sustainable development and the net-zero commitment imposed by the United Nations have become the subject of various research and emerging eco-friendly technologies worldwide. The principles of two concepts have also expanded to geotechnical engineering, where innovative biological-based techniques were found promising in future development. Vegetation as a genuinely compatible element with the environment plays a crucial role in ecological restoration and rehabilitation efforts through offering numerous environmental benefits. Previous research proved that plant root system and its hydrological interactions with soil and atmosphere can effectively modify the engineering properties of soils. The alterations induced by plant influence highlight vegetation as a widely embraced method for slope stabilization. To conduct a comprehensive examination, vegetation is contrasted with traditional construction techniques, including nailing and anchorage. This comparative analysis consists of two stages. Initially, the evaluation of slope stability is carried out using a numerical model across various slope geometries, with a specific focus

on the impact of the 10-year return rainfall. In the second stage, the environmental and economic aspects are assessed. This involves the utilization of life cycle assessment (LCA) and life cycle cost (LCC) analyses to ensure a comprehensive evaluation. According to a calibrated numerical model, it has been determined that vegetated slopes, up to a specific height of 8 meters, can effectively stabilize the slope, irrespective of the slope angle. Under these circumstances, even negative carbon emission can be achieved, attributed to the carbon-absorbing capacity of plants. For heights exceeding 8 meters, the recommendation is to employ traditional stabilization methods. For slopes with a moderate angle (30°-60°), the preference is for anchored method, primarily due to reduced carbon emissions resulting from the use of fewer elements. With an increasing number of elements, a preference for the nailed slope emerges. This choice is driven by the observation that as the number of elements in an anchored slope rises, the associated carbon emissions surpass those of a nailed slope, owing to the utilization of materials with higher carbon emissions. The main contributors to carbon emissions in the nailed and anchored slopes were steel bars and cement. In an economic evaluation, vegetation emerges as the most cost-effective method, and, in general, the nailing method proves to be less expensive than anchoring. The findings of this study highlight the effectiveness of integrating vegetation-based approaches in reducing carbon emissions and enhancing the environmental sustainability.

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MS13 / 936

Coarse-grained modeling of fluid transport in swelling porous media

Author: Jian Wu[1]

Co-authors: Yixiang Gan [1]; Pengyu Huang [2]; Luming Shen [1]

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Fluids can induce solid adsorption and swelling in porous materials when they infiltrate pores. For example, alkaline liquids created after water mixing with alkali metals can react with minerals like quartz or feldspar and form a new substance called alkali calcium silicate hydrate. Fluid flow facilitates the damage of concrete as this new substance can swell upon adsorbing water and crack the concrete. In carbon sequestration, CO2 injectivity can significantly decrease with time as gas adsorption induces swelling of the rock matrix and reduces pore spaces for the flow pathway. However, the coupling between fluid flow and solid deformation remains challenging to be captured by

numerical models.
Coarse-grained molecular dynamics (CGMD) bridges nano- and micro-scales by mapping a group of atoms/molecules into a single coarse-grained (CG) particle. Compared with all-atomic molecular dynamics (MD), it overcomes the difficulty of simulating multiphase flow with multiphysics in complex pore networks. This study introduces a novel CGMD model to achieve the coupling between fluid transport and solid deformation at the microscale. This model accurately simulates the interactions between fluids and solids, and between fluids and solids themselves. The solid comprises bead-spring chain networks considering bonding and non-bonding interactions and reproduces a broad range of Young's moduli and swelling ratios. The fluid is modeled by dissipative particle dynamics (DPD) and calibrated against density and viscosity at different pressures.
The proposed CGMD model has been adopted to study fluid transport through deformable and non-deformable nanochannels of varying sizes (35.4 nm~123.9 nm) and a simplified nanoporous medium composed of spherical solids. The results are analyzed using the Hagen-Poiseuille equation and the Kozeny-Carmen equation for validation. The effect of swelling on reducing fluid permeability is justified, and a relationship is established between fluid permeability and solid swelling. This study provides a straightforward new approach to modeling fluid transport in swelling porous media at the microscale within the framework of CGMD, with potential applications in concrete design and energy storage technologies.

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Poster / 940

Machine-learning-based forecasting model for nanoparticles controlling oil-water interface performance

Author: Dongming Li[1]

Co-authors: Bin Yuan [1]; Mingliang Han [1]; Wei Zhang [1]

[1] 中国石油大学（华东）

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Active nanofluids are colloidal systems composed of water-based active nanoparticles, garnering significant attention for their outstanding performance in enhancing the recovery efficiency of ultra-low permeability oil reservoirs. Currently, the mechanisms underlying the adsorption and oil film detachment at the oil-water interface by active nanoparticles remain unclear. Simultaneously, the lack of precise and efficient methods for the design and performance prediction of nanoparticle materials constitutes the core issue inhibiting the enhanced oil recovery potential of active nanofluids.. This study aims to dissect the behavioral rules of active nanoparticles at the oil-water interface and establish a predictive model for the interface-regulating performance of nanoparticles.
Conducted molecular dynamics simulations to investigate the adsorption and oil film detachment rules of active nanoparticles at the oil-water interface, introducing the binding energy ratio for the

evaluation of adsorption contact angles. Concurrently examined the influence of different oil phase components on the regulatory rules of nanoparticle behavior at the interface and established a quantitative relationship between adsorption contact angles and oil film detachment effects. Utilizing the aforementioned simulation methodology, constructed a database of nanoparticle-regulated oil-water interface samples. Subsequently, trained an artificial neural network model, establishing a machine learning-based predictive model for the interface-regulating performance of nanoparticles.
The simulation results dissected the regularities of adsorption and oil film detachment of active nanoparticles at the oil-water interface, offering guidance for the design of active nanoparticles. The adsorption and oil-stripping effects were found to increase initially and then exhibit a diminishing trend with the augmentation of alkane chain length and density. Through the training of a neural network on a sample database, a machine learning-based predictive model for the interface-regulating performance of nanoparticles was established. Predictive comparisons with practical examples validated the model's effectiveness and accuracy. The model is designed to investigate and predict the adsorption and oil-stripping effects of active nanoparticles at the oil-water interface.
The primary significance of this study lies in the coupling of molecular dynamics simulations with machine learning, dissecting the behavioral rules of active nanoparticles at the oil-water interface. Simultaneously, it establishes a predictive model for the interface-regulating performance of active nanoparticles. This work is poised to facilitate the application of active nanoparticles in enhancing oil recovery in ultra-low permeability reservoirs, enabling more effective decision-making in oil displacement and recovery strategies.

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941

Hybrid Modeling of Multiscale Gas Flow in Shale Digital Rocks

Authors: Dongchen Liu[1]; Jianfa Wu[1]; Deliang Zhang[1]; Chaozhong Qin[2]; Chao Luo[1]; Shuai Wu[1]; Rui Jiang[1]; Chongjiu Qu[1]; Meixuan Yin[1]

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The FIB-SEM imaging technique has opened the door to understanding the pore structure of shale. However, a large portion of subresolution pores of a few nano meters still challenge the modeling of gas flow capacity. In this work, the pore-size distribution information by low pressure gas (N2 and CO2) adsorption tests is integrated to a FIB-SEM digital shale core, and the controlling effect of subresolution pores on permeability is extensively studied by using a pore-network-continuum

hybrid model. Our results show that the connectivity of resolved pores by FIB-SEM is poor. The core permeability is mainly determined by subresolution pores with the pore sizes between 2 nm and 5 nm. By using the proposed pore-network-continuum hybrid model to respectively describe the flows in FIB-SEM resolved pores and subresolution pores, we can accurately calculate the shale permeability, and advance the digital core analysis of shale gas flow. This is of great significance for reservoir evaluation and production rule evaluation of shale gas reservoirs.

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Poster / **942**

An Autonomous Adaptive Meta Model (AAMM) for Real-Time Oil Rate Prediction and Optimization in Dynamic Environments

Authors: Fatna Said Adinani[1]; Kai Zhang[2]; Huaqing Zhang[1]; Johnson Joachim Kasali[3]

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

[2] *China University of Petroleum (East China); Qingdao University of Technology*

[3] *China University of Petroleum, Beijing*

This study introduces a groundbreaking Autonomous Adaptive Meta Model (AAMM) as an innovative solution to meet the escalating demand for precise and reliable oil prediction rates over a 20-year horizon. By leveraging machine learning algorithms and edge computing techniques, the AAMM dynamically adapts and optimizes its prediction model in real-time, responding to changing oilfield conditions. It integrates Extremely Gradient Boosting (XGBoost), Random Forest (RF), Bidirectional Long Short-Term Memory (BiLSTM), and Artificial Neural Network (ANN) to autonomously learn and adjust its parameters based on real-time feedback from the oilfield data. This adaptive capability enhances the predictive accuracy and reliability in dynamic and complex oilfield environments. Additionally, the AAMM incorporates edge-computing technologies to process and analyze data directly at the source to reduce latency and expedite decision-making. Utilizing a comprehensive dataset comprising historical oil production data, geological information, well characteristics, and other relevant factors, the AAMM remains up-to-date with the latest information through real-time integration of streaming data. Validation and test on real-world oilfield data demonstrate the AAMM's superiority over the traditional standalone models and static meta models. It's autonomous adaptation is proved crucial in maintaining accuracy midst changing conditions, providing a robust solution for oil production optimization.

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947

Principles of Shale Acidizing Reservoir Transformation Technology

Author: xuesong Li[None]

Co-authors: Ning Qi [1]; Xuhang Su ; Yixin Lu [2]

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

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

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Compared to conventional hydraulic fracturing reservoir reforming techniques, acid fracturing emerges as a promising alternative due to its remarkable permeability enhancement effects, reduced difficulty in fracturing deep shale formations, enhanced propensity for intricate seam network formation, and effective propping without the need for proppant. This comprehensive review presents an in-depth analysis of the existing literature on shale acidizing.

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Opening Ceremony

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Award Ceremony I

MS06-A / 950

Experimental study on hysteresis during cyclic injection in hierarchical porous media

Authors: Shuo Yang[1]; Si Suo[2]; Johan Revstedt[1]; Yixiang Gan[3]; Lei Wang[1]; Shervin Bagheri[4]

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Hydrogen (H_2) energy is being developed as a promising alternative to fossil fuels in response to growing energy demand and the urgent need to mitigate climate change. However, the significant obstacle to its wide application is the storage problem. Underground hydrogen storage (UHS) in depleted hydrocarbon fields and aquifers underground holds great promise. UHS includes temporary storage and later-on extraction (use) processes, corresponding to alternating displacement of hydrogen injection (drainage) and withdrawal (waterflooding). In UHS, a certain quantity of H_2 may be inevitably lost due to residual trapping. Throughout the cyclic injection process, the trapped H_2 might reconnect owing to hysteresis of saturation (Wang, Pereira, Sauret, & Gan, 2023) and relative permeability (Lysyy, Føyen, Johannesen, Fernø, & Ersland, 2022). Therefore, hysteresis effect during gas-liquid cyclic injection in porous media play an important role in application of UHS. Most current research efforts have primarily concentrated on cyclic injection in uniform porous media. However, in natural subsurface rock formations, porous structures typically exhibit multiple levels of pore sizes. There is an absence of experimental studies on the pore-scale mechanism by which geometry affects saturation hysteresis in the existing literature. In this work, based on 3D printing technology, we designed and fabricated the hierarchically structured porous media chip with dual permeability. Gas-liquid cyclic injection in uniform and hierarchical chips was studied by a high-speed imaging system emphasizing the impact of hierarchical structure on invasion behavior. The fingering morphology illustrates preferential invasion in 1^{s}t-order structure and significant capillary trapping in 2^{n}d-order structure, which are reconfirmed by phase saturation at each level of the hierarchical structure. The hysteresis effect was quantified based on Land model, and the result shows weaker saturation hysteresis effect during cyclic injection in hierarchical structure compared with uniform structure. To explore the causes, ganglion mobilization was investigated. Unlike uniform structures, inhibition of ganglion mobilization was observed in the hierarchical structure. Through the analysis of local invasion behavior, the connect-jump invasion method is identified as the primary reason for this suppression. Further, the mechanism behind the hysteresis difference was uncovered from two aspects: topology connectivity assessed by measuring normalized Euler number and relative permeability estimated by employing Lattice Boltzmann method (LBM). The results show the hierarchical structure has higher connectivity and relative permeability, which helps explain its limited hysteresis effect. The findings in this study enhance the understanding of the hysteresis effect when optimizing strategies for storage and extraction in Underground Hydrogen Storage (UHS).

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1 Z. Wang, J.-M. Pereira, E. Sauret, Y. Gan, Wettability impacts residual trapping of immiscible fluids during cyclic injection, Journal of Fluid Mechanics, 961 (2023) A19. 2 M. Lysyy, T. Føyen, E.B. Johannesen, M. Fernø, G. Ersland, Hydrogen relative permeability hysteresis in underground storage, Geophysical Research Letters, 49(17) (2022) e2022GL100364.

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Investigating Aquifer Thermal Energy Storage in the Texas Carrizo-Wilcox Aquifer using Numerical Simulations

Author: Ipsita Gupta[1]

Co-author: Richard Budiman [2]

[1] *LSU Professor*

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Aquifer Thermal Energy Storage (ATES) is an innovative and newly implemented geothermal technology in the US to mitigate global warming and reduce carbon emission from convention energy source generation. The technology was first put in place in Europe around 20 years ago, particularly in the Netherlands. ATES works by injecting warm water during summer and cold-water during winter.

The Texas Carrizo- Wilcox Aquifer is predominantly composed of brackish aquifers underlying fresh aquifers that can potentially be used to develop ATES without interfering with the existing fresh groundwater supply. The temperature range in this aquifer varies from 60℃ to 80℃ all year long which makes it attractive particularly for space-heating and greenhouse farming purposes. Numerical studies are conducted using SUTRA (Saturated-Unsaturated Transport) simulation software from USGS. Steady-state and transient models of Carrizo-Wilcox Aquifer are constructed and simulated with different set of variables to analyze the effects of several parameters such as well location, flow rates, boundary conditions, cyclic durations, as well as multi-well system utilizing dual aquifer layers in heat energy storage and production. Simulations show that injection, rest, and production period together with the flow rates are the most prominent factors affecting the thermal recovery efficiency in this study. The highest thermal efficiency is obtained by separating the injection and production well into different aquifer layers ensuring the temperature isolation between the two wells. This efficacy is attributed to the complete isolation of fluid temperature from the injection well, preventing any thermal degradation at production well resulting from cold fluid injection. The research demonstrates the feasibility of geothermal energy implementation in areas where high temperatures are not readily available. The results from this study can facilitate other studies for investigation into green geothermal energy resources in the US.

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Experimental investigation of fractured caprock breakthrough pressure under different proportions of sequestered gas conditions

Authors: Chuanjin Yao[None]; Xiuqing Zhang[None]; Yuyuan Song[None]; Jia Zhao[None]; Yiran Zhou[None]

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CO2 geological storage technology is an important means of mitigating the greenhouse effect, and reducing the risk of caprock leakage is a prerequisite for ensuring safe and efficient CO2 storage. In the process of storage, the fluctuation of underground pressure and the change of the original water-rock equilibrium will lead to the destruction of the caprock, thereby inducing the creation of cracks and subsequently increasing the risk of caprock leakage, which is a serious threat to the safety of groundwater and human. In order to ensure the safety of CO2 geological storage, it is particularly important to evaluate the leakage risk of the caprock, and breakthrough pressure is the most intuitive and effective parameter for caprock safety evaluation. In this study, the effect of different proportions of sequestered gas on the breakthrough pressure of fractured caprock is systematically discussed through step-by-step experiments. The experimental results show that the breakthrough pressure of the gas mixture of N2 and CO2 was greater than that of the gas mixture of CH4 and CO2, and the breakthrough pressure decreased with the increase of the molar percentage of CO2 in the gas mixture, which is due to the interfacial tension between CO2 and caprock fluid is the smallest, and it is easiest for gas seepage to occur. And the smaller the dip angle between the crack and the horizontal lamination of the caprock, the higher the breakthrough pressure and the lower the risk of CO2 leakage. This study can provide theoretical support for the safe implementation and leakage risk assessment of CO2 geological storage engineering.

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957

Relative motion of fluid flow in poroelasticity: Implication for cancellous bone

Author: Young June Yoon[1]

[1] *Hanyang University*

Corresponding Author: yoon05297@gmail.com

In porous materials, ultrasound propagates in two forms, namely fast and slow waves. The fast and slow waves are described by the bulk equation and poroelastic dynamic equation, respectively. In cancellous bone, the relative motion between the solid bone matrix and fluid is believed to generate slow waves. This paper explains the slow wave generation numerically.

Previous papers suggested that the fast wave of ultrasound penetrates through cancellous bone and passes through the solid bone matrix, and that the relative motion between the solid bone matrix and pore fluid generates the slow wave of ultrasound. The results of this study show that the relative motion between the solid bone matrix and pore fluid generated the slow wave of ultrasound in cancellous bone. Poroelastic calculation shows that the relative motion is exactly same as the second wave propagation.

Relative motion is very important in bone cell communication because the relative motion induces the shear stress on the bone membrane surface. However, high-frequency wave propagation holds the fluid flow because of fluid inertia. Thus, this result is for low-frequency wave propagation and induces the bone fluid flow inside the cancellous porous spaces.

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958

Why does bone respond to high-frequency stimuli?

Author: Young June Yoon[1]

[1] *Hanyang University*

Corresponding Author: yoon05297@gmail.com

Bone responds to low-amplitude high-frequency mechanical stimuli, but the underlying mechanism is not clear. Here, we explain the mechanism in terms of charged ions and poroelasticity. Charged

ions accumulate on the surface of a cancellous bone matrix when a low-magnitude high-frequency stimulus, and they attract osteoblasts and cause their aggregation on the bone matrix surface.
The ultrasound generates two longitudinal waves- fast and slow compressional waves in porous materials. Charged ions accumulate on the surface of the trabecula because of the fast compressional wave. The charge density increased significantly with an increase in the frequency and a decrease in the wavenumber. While the slow compressional wave causes the relative motion between the solid matrix and fluid in pores, the fast compressional wave goes through as the solid bone matrix is stationary with fluid. High-frequency mechanical stimuli induces only a small amount of relative motion between the solid matrix and fluid in pores because of the fluid's inertia. Thus, high-frequency mechanical stimuli mainly generate the fast compressional wave in the cancellous bone.
Let us suppose that positively charged ions are present on the surface of cancellous bone. In this case, a large number of osteoblasts attracts on the surface of the cancellous bone, similar to the case where a positively charged hydrogel on the surface of cancellous bone attracts a large number of osteoblasts to the surface. However, there is a need to clarify whether the calculated charge density is positive or negative. Negative charges promote osteopontin production and thereby inhibit hydroxyapatite crystallite growth.

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Characteristics of pore-fracture structure of anthracite reservoir in the southern Qinshui Basin, China

Author: Shiqi 世奇[1]

Co-author: Shuxun Sang [1]

[1] *China University of Mining and Technology*

Corresponding Authors: liushiqi@cumt.edu.cn, shxsang@cumt.edu.cn

The structural characteristics and topological properties of the coal seam pore-fracture network is a key scientific issue that urgently needs to be addressed in coalbed methane (CBM) development, which control the continuous process of CH4 adsorption/desorption-diffusion-seepage-production in the coal seam. Taking the Fanzhuang and Zhengzhuang block in the southern Qinshui Basin, China as an example, based on the X-ray CT scanning and FIB-SEM scanning results, the three-dimensional digital characterization and modeling methods of coal structure are applied to construct a three-dimensional digital structure relationship model of micro-nano-scale pore-fracture network in anthracite, and the development characteristics, genesis types, and connectivity of the pores and fractures in anthracite are discussed. The results indicate that the pore volume of anthracite in the southern Qinshui Basin is mainly composed of macropores and micropores, while mesopores are underdeveloped, which constrain the connectivity between macropores and micropores. There are exogenous macro-fractures, endogenous macro-fractures (cleats), and microfractures in anthracite.

The macro-fractures are relatively developed, with 2-3 stages visible, while the microfractures are widely developed, improving the connectivity of micro-scale pore-fracture network. There are two genesis types of pores in anthracite, which are metamorphic pores, common secondary gas pores, differential shrinkage pores, and macromolecular structural pores, and mineral-related pores, primarily including dissolution pores and intergranular pores. The macropores are mainly composed of microfrcture and secondary gas pores, the development degree of mesopores depends on the differential shrinkage pores and ultra-microfractures, while micropores are mainly macromolecular structural pores. The pores cross-section of anthracite in the southern Qinshui Basin is mainly irregular in shape, with significant capillary resistance. The pores have good connectivity, with various connectivity pathways, which are conducive to gas migration and production. However, with the decreases of the pore-fracture scale, the connectivity and permeability of pore-fracture decrease accordingly. Ultra-microfractures (including differential shrinkage pores), microfractures, and cleats play a major role in coal connectivity. Cleats are the main connected fractures at the micrometer to millimeter scale, microfractures are the main connected fractures at the micrometer scale, while differential shrinkage pores and ultra-microfractures are the main connected pores and fractures at the nanometer scale. In comparison to the Fanzhuang block, the development of mesopores (differential shrinkage pores and ultra-microfractures) in the Zhengzhuang block is poorer, resulting in lower connectivity at the micro-nano scale of pore-fracture networks, which may be related to the temperature and rustal stress during the thermal maturation phase, negatively impacting the CBM recoverability in the Zhengzhuang block.

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Plenary/Invited / 961

What is the co-moving velocity and why should we care?

Author: Alex Hansen[1]

[1] *NTNU*

Corresponding Author: alex.hansen@ntnu.no

When two immiscible fluids move through the same pore space, they interact. It is therefore hard to believe that the relative permeabilities describing the mobility of each fluid should be independent of each other. Yet, ever since 1936 when the concept of relative permeability was born, they have been treated that way. It is the aim of this talk to demonstrate that the intuition however is correct; they are indeed related. To do so, I introduce the co-moving velocity [1-8]. This is the average velocity change of the immiscible fluids when the average fluid velocity changes.

It turns out that plotted against the derivative of the average seepage velocity with respect to the saturation, it is a straight line. This result translates into a differential equation relating the two relative permeabilities. In clear language: Knowing one, we know the other.

I will explain why the co-moving velocity is linear in the derivative of the average seepage velocity. What I cannot explain at this point is why it is so insensitive to the parameters describing the flow [8].

The relative permeability approach is valid as long as the capillary number does not enter as a parameter affecting the relative permeabilities. The validity of the theory behind the co-moving velocity goes beyond this constraint. I will discuss this non-linear flow regime and the co-moving velocity also in this context.

Lastly, I will explain how the co-moving velocity is an example of a new class of variables in the thermodynamics of mixtures.

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Plenary/Invited / 962

Inertia, non-equilibrium, and momentum conservation in porous media

Author: Ivan Lunati[1]

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Theoretical and computational models of flow through porous media typically ignore inertial effects and use Darcy's law (and extensions thereof) to approximate momentum balance. This contrasts with experimental observations of rapid fluid movement in the pore space, such as Haines jumps

that occur in presence of multiple flowing phases. Also, neglecting acceleration may lead to contradictions analogous to those encountered when Fourier's law is used as constitutive equation in the heat equation.

We review the role of local inertial effects in shaping the morphology of invading fluid fronts, paying particular attention to the effects of surface energy instabilities, spontaneous reconfiguration of the interface, collective pore filling, and hysteresis. Then, we discuss how a macroscopic momentum-balance equation can be introduced to model multiphase flow in porous media and describe salient flow features that are observed in the experiments but cannot be captured if Darcy's law is used.

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Advanced multi-scale and multi-modal 3D imaging and modelling of porous anode microarchitecture and shape changes in rechargeable zinc-based batteries

Author: Lucia Mancini[None]

Corresponding Author: lucia.mancini@zag.si

The increasing need of reliable and sustainable energy supply, storage and portability, combined with global industrial competition, imposes a stringent schedule for battery research and development. Among the different technologies available nowadays, rechargeable zinc-based batteries are promising candidates owing to their comparatively high specific energy, abundant and distributed raw-material resources, moderate cost, environmental friendless and safety. The successful applications of rechargeable Zn batteries are still hindered by various technical pitfalls, a crucial one being their limited cycle life due to uncontrolled morphological changes of the anode upon applying discharge/charge cycles. The textural and geometrical properties of the pore network, including pore size distribution, shape, connectivity and tortuosity, as well as the anode shape changes brought about by cycling, play a crucial role in ionic transport in batteries and electrolyte flow in particulate-anodes, controlling their final electrochemical properties. These properties depend on the anode microstructure, electrolyte composition, use of chemical additives and are a function of the power applied to the battery, representing significant challenges for battery characterization and energy storage applications. An accurate estimation of the percolating networks of ionic conductors and fluid transport properties in the porous electrode material is essential to decipher the battery performance in terms of capacity loss when cycling and can be derived through the integration of optimized anode manufacturing processes, electrochemical characterization and morpho-textural analyses of the battery components and assembled cells. The recent advances in X-ray and neutron 3D imaging techniques, in static and dynamic conditions, through a multi-scale approach coupled with computational modelling simulating the cycling behaviour of batteries, can offer a deeper understanding

of how the pore network properties influence fluid transport and their impact on the battery operation.
In this talk the result of investigation of Zn-based batteries cycling for traditional and innovative electrolyte chemistries and electrode configurations, at current densities and depths of discharge of practical interest, will be presented.

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Validating computational models for carbon storage

Author: Jan Nordbotten[None]

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As is common for subsurface applications, the planning and operation of geological carbon storage relies heavily on computational models. Arguably, several decades of experience from the extraction of subsurface resources support the validity of these tools, in particular during the active carbon dioxide injection and early post-injection phase. However, validation of long-term carbon storage performance, on the time-scales of hundreds of years after injection, cannot directly be justified by either existing engineering practice nor natural analogues.

The FluidFlower validation and forecasting study was specifically designed to provide validation data for carbon storage. Moreover, by conducting a multi-institutional and multidisciplinary double-blind study, we were able to address the forecasting skill of the carbon storage simulation community. In this talk we give an overview of the results of the study, both from the perspective of model validation and assessment of forecasting skill.

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Plenary/Invited / **965**

Orthogonally different mineral reactions, same outcome of permeability reduction: How can this be?

Author: Catherine Peters[None]

Corresponding Author: cap@princeton.edu

Sustainable energy technologies that involve subsurface gas storage require reliable containment of buoyant fluids. An example is geologic carbon sequestration in which large volumes of CO2 are injected deep underground into porous formations with overlying caprocks. Storage security could be jeopardized if fractures exist, so strategies are needed to seal permeable flow paths. In our work, two orthogonally different mineral reaction scenarios were explored. In one case minerals precipitated and in the other case minerals dissolved, but both cases had the same outcome of reduced fracture permeability. How can this be? In the first case, vein minerals from a mudrock sample of the Wolfcamp formation provided insights about syntaxial mineral growth in a fracture. Dolomite and other carbonate minerals had precipitated in the fracture, closing it off to fluid flow. In the second case, a carbonate-rich shale was reacted leading to calcite dissolution along fracture surfaces. Subsequent compression from normal stress collapsed the altered layer, sealing the fracture and reducing permeability. These studies show that multiple mineral reaction mechanisms can achieve fracture sealing and permeability reduction, a favorable outcome in subsurface applications where the goal is to reduce leakage risks.

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Plenary/Invited / **966**

Property-Preserving Schemes for Porous Media Flow: Phase-Wise Conservation, Bound Preservation, and Energy Stability

Author: Shuyu Sun[None]

Corresponding Author: shuyu.sun@kaust.edu.sa

Single-phase and multi-phase flow and transport in porous media are central to a wide range of natural and industrial processes, including geologic CO2 sequestration, enhanced oil recovery, and

water infiltration into soil. Petroleum engineers use reservoir simulation models to manage existing petroleum fields and to develop new oil and gas reservoirs, while environmental scientists use subsurface flow and transport models to investigate and compare for example various schemes to inject and store CO2 in subsurface geological formations, such as depleted reservoirs and deep saline aquifers. One basic requirement for accurate modeling and simulation of multiphase flow is to have the predicted physical quantities sit within a physically meaningful range. For example, the predicated saturation should sit between 0 and 1 while the predicated molar concentration should sit between 0 and the maximum value allowed by the equation of state. Unfortunately, popular simulation methods used in petroleum industries do not preserve physical bounds. A commonly used fix to this problem is to simply apply a cut-off operator. However, this cut-off practice does not only destroy the local mass conservation but it also damages the global mass conservation, which seriously ruins the numerical accuracy and physical interpretability of the simulation results. Another major issue with common algorithms for two-phase flow, especially common semi-implicit algorithms, is that they are (locally) conservative to just one phase only, not all phases. Moreover, stability of the algorithms has been shown to be crucial to certain multiphase flow scenarios.
In this talk we present our work on both fully implicit and semi-implicit algorithms for two-phase and multi-phase flow in porous media with capillary pressure. Our proposed algorithms are locally mass conservative for all phases. They are able to accurately reproduce the discontinuity of saturation due to different capillary pressure functions, and they enjoy the merit that the total velocity is continuous in the normal direction. Moreover, the new schemes are unbiased with regard to the phases and the saturations of all phases are bounds-preserving (if the time step size is smaller than a certain value for semi-implicit algorithms). We also present some interesting examples to demonstrate the efficiency and robustness of the new algorithms. The semi-implicit algorithms are based on our novel splitting of variables, and the fully implicit algorithms are based on the two nonlinear preconditioners of active-set reduced-space method and nonlinear elimination, as well as the linear preconditioner of overlapping additive Schwarz type domain decomposition. The semi-implicit part of this presentation is based on our joint work with Huangxin Chen (Xiamen University), Jisheng Kou (Shaoxing University), Xiaolin Fan (Guizhou Normal University), and Tao Zhang (KAUST), and the fully implicit part is based on our joint work with Haijian Yang (Hunan University), Chao Yang (Beijing University), and Yiteng Li (KAUST).

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Plenary/Invited / **967**

Simulating flow and solute transport in subsurface environments: From pore-scale to beyond

Author: Xiaofan Yang[None]

Corresponding Author: xfyang@bnu.edu.cn

Research of the multi-scale, multi-phase, and multi-processes system is of great interest in understanding subsurface environments. However, the coupled flow and transport processes are complex

yet challenging for model development and utilization. There have been numerous object-oriented and easy-to-use models/codes across scales to facilitate consistency, continuity, and reproducibility in subsurface research. In addition, pioneer efforts on upscaling also inspire the development of hybrid multi-scale models. It is then critical to intercompare codes and approaches for their evaluation or validation, and propel discussions for optimizing the codes and the development of the next-generation numerical approaches. In this talk, we present a suite of at-scale and multi-scale models that we developed and utilized in recent years for simulating flow and transport processes, with intercomparison and benchmarking cases, including: (1) pore-scale models for simulating flow, solute transport and biofilm growth in porous media; (2) Darcy-scale models for simulating thermo-hydrological processes in frozen soils; (3) regional-scale groundwater models for simulating groundwater-surface interactions; (4) hybrid multi-scale models (pore- to Darcy-scale) for numerical upscaling.

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Plenary/Invited / 968

Physical Insights into Phase Transition and Capillary Transport in Porous Media with In-situ NMR-MRI Characterization

Author: TieJun (TJ) Zhang[None]

Corresponding Author: tiejun.zhang@ku.ac.ae

Interfacial transport and phase transition are essential for a large variety of energy and sustainability applications, while in-situ characterization provides instrumental ways of probing and enhancing thermal-fluid transport in porous media. In this talk, I will share our recent progresses on water evaporation and ice melting in homogeneous and heterogeneous opaque porous media, by utilizing non-destructive nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI). By characterizing the amplitude variation of NMR transverse relaxation time T2, we find that cavitation occurs across the entire porous media along with the water evaporation from open surface. Disconnected void clusters at different depths in the porous medium are also observed from MRI scanning and optical images. These evidences confirm the occurrence of cavitation in porous media because the water is stretched to metastable state by large capillary pressure from the evaporating meniscus. Moreover, transient T2 distributions from NMR enable us to reveal the substantial role of inherent throat and pore confinements in ice melting among various porous media. The increase in minimum T2 offers new findings on how the confinement between ice crystal and particle surface evolves inside the pores of mushy zone. The evolution of melting front and 3D spatial distribution of water content are directly visualized by a stack of temporal cross-section images from MRI, in consistency with the associated NMR results. For heterogeneous porous media like lunar regolith simulant, the T2 curves show two distinct pore size distributions with different pore-scale melting dynamics, and the maximum T2 keeps increasing throughout the whole ice melting process instead of reaching steady for homogeneous porous media. These transport and phase change physics opens up new

avenues to develop novel solutions for water-energy-food nexus and in-situ resource utilization towards deep space exploration.

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Plenary/Invited / 969

Reservoir Simulator Development: The Past, Present and Future

Author: Zhangxing (John) Chen[None]

Corresponding Author: zhachen@ucalgary.ca

Reservoir simulators have been developed in the past 70 years. They have been widely used to predict, understand, and optimize complex physical processes in modeling and simulation of multiphase fluid flow in petroleum reservoirs. These simulators are important for understanding the fate and transport of chemical species and heat and maximizing the economic and environmental performance of exploration and production of fossil fuel energy.

The development of reservoir simulators has been concentrated on conventional oil and gas reservoirs in the last century, and efficient black oil, compositional and thermal simulators have been successful in their application to the recovery of conventional oil and gas resources. As these conventional resources dwindle, the recovery of unconventional oil and gas (such as heavy oil, oil sands, tight and shale oil and gas, and coalbed methane) resources is now at the center stage. While the development of unconventional reservoir simulators has been focused on in this century, a lot of challenges still exist because of the significant differences between conventional and unconventional reservoirs in their multi-scale phenomena, fluid occurrence states, flow mechanisms, and production technologies.

The speaker has engaged in the development of reservoir simulators for over 30 years. His group has developed parallel and intelligent simulators that can efficiently simulate complex fluid flow problems with giga (billion) grid block cells and reduce simulation time from days to seconds. For over ten years, his group has also incorporated artificial intelligence (AI) and quantum computing algorithms into these reservoir simulators. Fast and accurate simulators can increase energy production due to full utilization of available data and better understanding of the chemical and physical mechanisms involved, process designs and uncertainty analyses. In this plenary presentation, the speaker will give an overview on the development of conventional and unconventional reservoir simulators, the incorporation of parallel and AI algorithms into these simulators, and the quantum computing potential to solve reservoir simulation problems. The present status, existing challenges, and future prospects on reservoir simulators will be emphasized in this plenary presentation.

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Plenary/Invited / 970

Chemistry and Application of Soft Porous Crystals

Author: Susumu Kitagawa[None]

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With the Industrial Revolution in the 19th century, humans began to create technologies that consume huge amounts of energy. Initially, people used solid coal as an energy resource. In the 20th century, the focus changed to liquid petroleum. In the 21st century, where the depletion of petroleum has become a critical concern, gases (e.g., natural gas and biogas, and even air) should play important roles—an "age of gas"is dawning. However, a gas is a form that is difficult to handle because it is easily dispersed, creates mixtures, has a low concentration under normal conditions, and is invisible. In particular, new porous materials are indispensable for advancing science and technology to control gases at will.
As the promising materials to address global issues of clean energy technologies and environmental sustainability, the emerging class of crystalline microporous materials, porous coordination polymers (PCPs) or metal-organic frameworks (MOFs), have been applied in fields of gas storage and separation, delivery vessel, sensors, catalysis, supercapacitors, FETs, batteries, proton conduction, and so on. We have found the 3rd generation (3G) PCPs/MOFs (Soft porous crystals, SPCs) that possess flexible or dynamic porous frameworks reversibly respond to external stimuli, not only chemical but also physical, unlike robust PCPs/MOFs (2G). In particular, by controlling the local motion of organic ligands that construct the framework, we discovered and developed an effective mechanism for separating gas mixtures with very similar properties, such as oxygen/argon, and light water/heavy water isotopologue mixtures.
This talk provides an essential and accessible overview of the chemistry of SPCs, their current features, and the outlook of further developed materials as 4th generation PCPs/MOFs which exhibit multi-functions simultaneously or alternately in combination.

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Plenary/Invited / **971**

Nanosized Zeolites with Exceptional Adsorption Properties

Author: Svetlana Mintova[None]

Corresponding Author: svetlana.mintova@ensicaen.fr

The transition of the global energy system from traditional fossil fuels to renewable and sustainable energy sources and processes necessitates the development of new materials and the reinvention of existing ones. Zeolites will play a key role in facilitating this transition due to their exceptional qualities, which make them valuable in essential catalytic and adsorption processes, such as carbon capture and storage. The zeolites used in these processes consist of micrometer-scale particles. Consequently, small molecules must diffuse a distance approximately tens of thousands of times their own size through the particles. This results in a relatively large mass transfer zone within a fixed bed configuration, limiting the usable capacity in separation processes.

Nanozeolites offer several key advantages over their conventional micron-sized counterparts, such as high surface-to-volume ratios that provide greater access to more active sites, rapid diffusion properties, and rich chemistry. Furthermore, the direct synthesis using inorganic structure-directing agents ensures the formation of nanozeolites with uniform elemental composition and desirable adsorption properties, eliminating the need for post-synthetic calcination treatment.

In this presentation, I will discuss the synthesis of nanosized zeolites with various sizes, morphologies, and framework structures by tailoring the crystallization process. The diffusion properties of the nanosized zeolites were studied through breakthrough curve analysis, revealing exceptionally sharp curves indicative of rapid diffusion due to the nanosized crystals and desired morphology. The unique adsorption properties of nanozeolites make them interesting candidates for gas separation applications in humid streams.

Acknowledgments:
This research was co-funded by the European Union (ERC, ZEOLIghT, 101054004). The views and opinions expressed are solely those of the author and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them. The author acknowledges the Label of Excellence: Centre for Zeolites and Nanoporous Materials supported by the Region of Normandy (CLEAR).

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Plenary/Invited / **972**

Multiscale Considerations on Porous Media Heat Transfer

Author: Changying Zhao[None]

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Heat transfer in porous media is ubiquitous in many industrial applications, such as heat exchangers, heat pipes, heat storage system, and porous coatings for thermal radiation. Thus, it is of great importance to understand in depth the heat transfer in porous media. This, however, is still a huge challenge, mainly attributed to the following fact. First, heat transfer in porous media is a process involving multi scales. The pores in porous media can be multi scales, ranging from nano to milli meters; and the heat transfer in each pore of porous media controls the continuum- (macro) scale heat transfer in porous media. Second, heat transfer in porous media include multiple interactions, e.g., the interaction at the interfaces between fluids and solid matrix of porous media in single phase convection, interaction at the interface between fluids of different phases in phage change heat transfer, and heat transfer between solid matrix in thermal radiation. Thus, a multi scale exploration, from interface- to pore- and continuum-scale, is needed so as to disclose in detail the mechanisms of heat transfer in porous media. In this talk, we will introduce our recent multi-scale studies on the sing-phase convection, phase change heat transfer, and thermal radiation in porous media. As for the single-phase convection, the thermal non-equilibrium effects in forced and natural convection in porous media are clarified from the pore- and continuum-scale perspectives; and the permeability for natural convection is discussed. As for the gas-liquid and liquid-solid phase change heat transfer in porous media, the movement of phase interfaces in the nano- and micro-pores of porous media is disclosed, and its effects on the continuum-scale heat transfer is revealed. As for the thermal radiation heat transfer in porous media, a multiscale framework is established, which can account for the dependent scattering effects at microscale and the coherent effects of multiple scattering at mesoscale; based on this framework, an accurate prediction of macroscale radiative properties of various densely packed porous media is achieved. Furthermore, the role of far-field and near-field interferences in the wave aspects of thermal radiation transfer is quantitatively revealed.

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MS09 / **973**

Motion of a viscous slug on heterogeneous surfaces

Author: Bauyrzhan Primkulov[1]

Co-authors: Amir Pahlavan [2]; Luis Cueto-Felgueroso [3]; Ruben Juanes [1]

[1] *MIT*

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Corresponding Authors: bprimkul@mit.edu, amir.pahlavan@yale.edu, luis.cueto@upm.es, juanes@mit.edu

We present a theoretical study of viscous slug motion inside a microscopically rough capillary tube, where pronounced stick–slip motion can emerge at slow displacement rates. The mathematical description of this intermittent motion can be reduced to a system of ordinary differential equations, which also describe the motion of a pendulum inside a fluid-filled rotating drum. We use this analogy to show that the stick–slip motion transitions to steady sliding at high displacement rates. We characterize this crossover with a simple scaling relation and show that the crossover is accompanied by a shift in the dominant energy dissipation mechanisms within the system.

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975

A semi-analytical method for multi-well system productivity decline under different bottom-hole flow pressure production conditions

Author: 玉胜翟[None]

Co-authors: erlong yang [1]; jin lv [1]

[1] *Northeast Petroleum University*

Corresponding Author: zys9932@163.com

In this paper, a numerical approximate analytical model is established for the production performance of a number of Wells in a closed rectangular reservoir with constant bottom-hole flow pressure. It is obtained by a series of mathematical methods such as superposition principle, Laplace transform, Dirac function, convolution theorem and Green function. The model is verified by reservoir numerical simulation software CMG. The results show that the model can predict the production performance of multi-well system under bottom-solid flow pressure in a closed rectangular reservoir quickly and accurately.

The results show that in a certain period of time, with the increase of the number of Wells and the decrease of the bottom hole pressure of adjacent Wells, the production of a single well decreases, while with the decrease of the bottom hole pressure of adjacent Wells, the total production of the reservoir increases. In a certain period of time, the greater the distance between the observation well and the adjacent well, the smaller the interference from the well, then the greater the output of the observation well and the cumulative output. The rate of production decline depends on the number of Wells, well spacing, production mode of adjacent Wells, opening time of adjacent Wells and reservoir scale.

Compared with the empirical or semi-analytical models in other literatures, the model proposed in

this paper is completely analytical and has a solid theoretical basis, which can accurately and quickly predict the production performance of multiple Wells under constant bottom-hole flow pressure.
Key words: multi-well system; Principle of superposition; Analytical model; Laplace transform; Green function

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Poster / 979

Connectivity of multiscale porous structures of shale rocks based on multiscale imaging analysis

Authors: Bowen Shi[1]; Chaozhong Qin[2]; Han Jiang[1]; Zhiwei Wang[1]

[1] 重庆大学

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Pore connectivity is a critical factor influencing the migration and production of shale gas (Sun et al., 2017). However, the inherent heterogeneity of shale, characterized by the development of various pore types (Loucks et al., 2012; Ma et al., 2017), renders the detailed and quantitative characterization of shale pore connectivity challenging (Zhao et al., 2020). The advancement of imaging technologies at different scales has facilitated the assessment of pore connectivity. In this study, we aim to investigate the pore structures and pore connectivity of the Longmaxi Formation shale in the Sichuan Basin. Imaging data include scanning electron microscope (SEM) and focused ion beam scanning electron microscopy (FIB-SEM). Machine learning algorithms were applied to shale image segmentation, revealing the development of distinct pore types. Additionally, high-pressure mercury intrusion and nitrogen adsorption experiments were employed to evaluate pore distributions and connectivity. The results demonstrate that machine learning-based image segmentation techniques effectively delineate various pore types on MAPS, including organic matter and clay ratios, as well as facial size characterization. The connectivity of organic matter pores is intricately linked to pore types, with honeycomb-like organic pores exhibiting the largest average pore diameter and good connectivity, followed by mixed organic pores. However, the latter lacks permeable channels at the FIB-SEM resolution. Sponge-like organic pores exhibit the poorest connectivity and porosity. Pores with a size smaller than 30 nm, which FIB-SEM cannot identify, significantly contribute to the connectivity of organic pores.

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Poster / 980

InPore: Image-based and GPU-Accelerated Volumetric Lattice Boltzmann Method for Pore-Scale Porous-media Flows with Applications

Author: Huidan Yu[1]

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Recently developed image-based computational fluid dynamics (ICFD) techniques have revolutionized the study of pore-scale porous media flows (PSPMFs) by allowing for simulations within realistic porous structures extracted directly from images. Pore-scale fluid dynamics delve into the fundamental physics governing flow, transport, reaction, adsorption, and deformation within heterogeneous porous materials, marking a significant leap towards establishing heterogeneous porous media flow as a standard analytical tool. The applications of this advancement are diverse and far-reaching, encompassing scenarios such as tracking chemical contaminant propagation in underground reservoirs, understanding ink permeation dynamics, modelling sedimentation processes, optimizing hazardous waste storage, and predicting fluid flow behaviours in oil reservoirs and biological tissues. Traditionally, porous media flow was approached through temporally and spatially averaged models, relying on phenomenological and empirically derived equations such as Darcy's law. However, these conventional methods often fell short in capturing the intrinsic complexity of porous media due to the lack of suitable research tools. In this context, we present InPore, a groundbreaking computational platform that employs a kinetic-based volumetric lattice Boltzmann method to solve PSPMFs within image-derived porous structures. InPore stands out for its integrated modelling approach, seamlessly combining image extraction and fluid dynamics simulation, thereby eliminating the need for additional grid or mesh generation steps and simplifying data transfer across software packages. Furthermore, InPore leverages state-of-the-art GPU (Graphic Processing Units) parallel computing technology to enable rapid and localized computations, facilitating high-fidelity simulations. During our presentation, we will showcase InPore's capabilities through application studies and discuss its integration with supplemental mechanisms such as mass/heat transfer, interfacial dynamics, and chemical reactions. These enhancements aim to broaden InPore's functionality for tackling real-world porous media flows, thereby advancing our understanding of intricate phenomena within porous materials.

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MS15 / **981**

Effect discussion and workflow establishment of machine learning algorithm in logging classification: A case study from the classification of sepiolite bearing strata in the first member of Maokou Formation

Author: 杉任[None]

Corresponding Author: raiten@foxmail.com

The carbonate reservoir in the first member of Maokou Formation (Maokou-1 Member) of Middle Permian in Sichuan Basin have the characteristics of self-generating and, self-storage. Maokou-1 Member is expected to become a new field of unconventional gas reservoir exploration in carbonate rocks. The organic matter and pore development of Maokou-1 Member carbonate rocks are closely related to sepiolite bearing strata. Aiming to predict the sepiolite bearing strata from logging data, with core observation, microscopic analysis, XRD analysis. After sensitivity analysis, CNL, DEN, GR, RT, RXO and AC logging curves are selected as features. To overcome the imbalance among different features, this work introduces SMOTE algorithm. Comparison of classification and content prediction for sepiolite bearing strata among CatBoost, XGBoost, LightGBM, random forest and ANN models indicates CatBoost has good performance in binary and multi classification and XGBoost has a good performance in the regression. The prediction process of sepiolite bearing strata is put forward. The prediction process of sepiolite bearing strata is as follows: (1) Binary classification via CatBoost to judge the existence of sepiolite bearing strata; (2) Multi classification via Catboost to discriminate the type of sepiolite bearing strata; (3) Regression via XGBoost to predict the talc content; (4) Using talc content to calculate effective thickness of sepiolite bearing strata in different types.

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982

Pore-scale multi-phase flow simulations: Challenges in modeling contact angle with the color gradient lattice Boltzmann method.

Authors: Fizza Zahid[1]; Jeffrey Cunningham[2]

[1] *University of Engineering & Technology Lahore*

[2] *University of South Florida*

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Simulations of multi-phase flow at the pore scale in porous media require accurate modeling of fluid and flow properties to depict realistic fluid behavior. One such property is the contact angle, which is defined as the angle formed at the interface where the fluid meniscus and the solid surface meet with each other (Blunt, 2017). Modeling of the contact angle is incorporated in simulations as a way of accounting for the wettability of the solid surface. A suitable contact angle algorithm specifies the contact angle, and it must be free from numerical artifacts such as distorted fluid transfer across the solid surface (Leclaire et al. 2016, Chen et al. 2019). The objective of this work is to understand the effect of fluid-fluid viscosity ratio on simulation of contact angles under various wettability boundary conditions in lattice Boltzmann simulations of multi-phase flow. We employed a color gradient model (Guntensen et al. 1991, Reis and Phillips, 2007) to simulate multi-phase flow at the pore scale. Two contact angle modeling algorithms are compared: the standard "virtual densities"approach (Latva Kokko and Rothman, 2005), and the geometric boundary condition (Xu et al. 2017). We performed a series of benchmarking tests for static contact-angle modeling and subsequent non-wetting phase fluid invasion (i.e., drainage) in a porous domain. In this presentation, we will summarize the strengths, weaknesses, and capabilities of the two algorithms considered. Moreover, the effect of viscosity ratio on accurately modeling contact angle is emphasized. Therefore, the results of this work can help lattice Boltzmann modelers to adopt the algorithm that is best suited for their application of interest.

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983

Managed Phreatic Zone Recharge for Irrigation and Wastewater Treatment

Authors: Darrell Tang[None]; Ruud Bartholomeus[1]

[1] *Wageningen University*

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Managed phreatic zone recharge with marginal water, using (existing) drainage systems, raises the water table and increases water availability for crops. This nature-based solution uses the soil, groundwater, and rainwater between the drains and root zone as a buffer zone for biodegradation and adsorption; due to biodegradation and adsorption, the soil functions as a bioreactor. This is a newly developed method of freshwater conservation and marginal water treatment and disposal, but risks crop and environmental contamination. The fate of contaminants of emerging concern (CECs) within the irrigated water is addressed. We introduce numerical and analytical models, inspired loosely by a field site where treated domestic wastewater is used for subsurface irrigation. The treated wastewater would otherwise have been discharged into rivers, thereby spreading downstream. Model results show that minimal amounts of CECs are transported to deeper aquifers. Crops are not contaminated, except during dry years where small amounts of mobile CECs rise to the root zone, but then only directly above each irrigation drain. Under an annual precipitation surplus, less-mobile solutes are thus unlikely to ever enter the root zone. The primary mechanism of solute transport is lateral advection within the phreatic aquifer. Despite spatio-temporal heterogeneity in water flux magnitudes and directions, contaminant retardation does not significantly alter mass balance outcomes, only how fast it gets there. Therefore, persistent CECs pose the greatest risks, though overall environmental and crop contamination risks appear low. To maximize complementarity with subsurface irrigation systems, future advances in water treatment technologies should focus on removing persistent CECs. However, the system may be unsuitable for climates with annual precipitation shortages, as CECs may accumulate in the root zone and crops.

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MS16 / 986

The effect of graphene and porous coatings on flow boiling in flat microchannels under intense localized heating

Author: Dmitry Zaitsev[1]

Co-authors: Andrey Semenov [1]; Maxim Pukhovoy [1]

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Subcooled water flow boiling experiments were carried out in flat mini- and microchannels under intense local heating (up to 1600 W/cm2) for different heater surface morphology. Two different heaters were used: 10x10 mm2 heater and 3x3 mm2 heater. In total, 4 different types of heating surfaces were used: 1) smooth copper, 2) rough copper, 3) porous coating, 4) graphene coating. The structure of surfaces was studied in detail using atomic force and electron microscopy methods, as well as spectroscopy Raman scattering of light. The DSA100 KRUSS automated measuring system was used to study wettability of the surfaces. In experiments on flow boiling it was found that with an increase in the channel height in the range of 0.2 –3.7 mm, the heat transfer rate and critical heat flux increases significantly. For a given fluid flow rate and channel height, the critical heat flux on the 3x3 mm2 heater exceeds the heat flux on the 10x10 mm2 heater, and with increasing channel height this difference increases. Boiling curves were obtained for different water flow rates at different channel heights for heaters measuring 3x3 and 10x10 mm2. The behavior of the boiling curves is generally similar for both heater sizes - over the entire range of water flow rates and channel heights. It was found that at high values of mass flow rate of water, the critical heat flux for porous surface exceeds by approximately 30% the critical heat flux for smooth surface. On porous surface the heat transfer coefficients are significantly higher than on smooth surface. Moreover, at relatively small values of overheating, the difference in the heat transfer coefficient is two times and more. A series of experiments were carried out to study the effect of the heater coating on the frequency of formation of vapor bubbles. It was found that at relatively low heat fluxes, the specific frequency of bubble formation on rough surface, and also on surface coated with graphene, is higher than on smooth one. However, as the heat flux increases, the difference in the frequency of bubble formation on these surfaces practically disappears. Whereas the formation of bubbles on the porous surface occurs with twice the frequency compared to other surfaces in the entire range of heat fluxes. The results obtained can explain the recorded significantly higher heat transfer coefficients and critical heat fluxes on the porous surface.

The work was supported by the Russian Science Foundation (grant no. 22-49-08018).

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Poster / 987

The wettability of surfactant solutions on particles in simulated reservoirs

Author: Wang Zheng[1]

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The study employed the Washburn capillary rise method to explore the wettability of three conventional cationic, anionic, and nonionic surfactants - CTAB, SDS, and TX-100 - on powders with varying polarities and the resultant behavior of droplets under capillary force. For kaolin, illite, and silica nanoparticles, CTAB's hydrophilic portion interacted with the powder through electrostatic forces. TX-100 molecules adhered to solid particles via hydrophilic epoxy groups and hydrogen bonding interactions. SDS molecules attached to hydrophilic particles through hydrophobic groups and Lifshitz-van der Waals interactions. Moreover, in the case of hydrophobic oil sands, CTAB, SDS, and TX-100 exhibited adsorption through hydrophobic interactions. Notably, at the critical micelle concentration (CMC), surfactant molecules aggregate to form micelles, impacting solution mobility and altering wetting properties such as contact angles. This study highlights the dynamic interplay between surfactant solution surface tension, solid-liquid interfacial tension, and their effects on wetting behavior at varying solution concentrations. The competitive relationship between dynamic adsorption and microscopic surface tension influences the wetting dynamics of the solution.

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Emulsion Flow in Porous Media

Author: Mkhitar Ovsepian[1]

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The global demand for oil continues to rise, requiring the optimization of hydrocarbon extraction from existing mature fields through advanced enhanced oil recovery (EOR) technologies. Emulsions offer a promising method to enhance oil recovery by modifying fluid interfacial properties. This work presents a comprehensive review of emulsion-based EOR, focusing on the emulsion behavior and efficacy in porous media and encompassing following aspects: (1) physical simulations of the emulsion flow in porous media in the lab, (2) in situ emulsion formation in porous media, (3) emulsion flow characteristics and factors influencing, (4) emulsion rheology in porous media, and (5) numerical modeling of emulsion flow in pores.

First, various laboratory techniques for studying emulsion flow, ranging from core flooding experiments to microscopic observations and imaging, are discussed, providing insights into emulsion behavior and its distribution within pore structures under controlled conditions, thereby aiding in the optimization of EOR strategies.

Then, the phenomenon of in situ emulsion formation within reservoirs and its underlying mechanisms, which involve oil snapping and emulsifier shearing, are elaborated. By elucidating the flow characteristics of in situ-formed emulsions and possible blockage mechanisms, we can gain a deeper understanding of their performance in porous media. Furthermore, the work explores the factors influencing emulsion flow dynamics, ranging from dispersion phase size and concentration to formation water salinity and pH.

Furthermore, a mathematical model for emulsion effective viscosity to capture this variability is described considering that the apparent viscosity of emulsions undergoes changes as it flows through porous media. A comprehensive understanding of the mechanisms governing emulsion viscosity in complex pore structures is essential to devise strategies to mitigate flow resistance and enhance oil recovery rates.

After understanding the characteristics of emulsions, we discuss numerical modeling approaches for simulating emulsion flow in porous media, including models such as the homogeneous model, droplet retardation model, filtration model, and capillary network model. These modeling tools facilitate the prediction of emulsion behavior under varying reservoir conditions, offering valuable insights for optimizing EOR operations.

In conclusion, this work sheds light on the intricate interactions between emulsions and porous media, providing valuable information and perspectives for further studies and efficient application of emulsion-based EOR methods.

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A pore-scale lattice Boltzmann model for solute transport cou-

pled with heterogeneous surface reactions and mineral dissolution

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In this paper, we propose a pore-scale lattice Boltzmann model to treat heterogeneous surface reactions coupled with mineral dissolution. The primary innovation lies in the transformation of surface reactions, originally treated as boundary conditions, into volume source terms through dimensionality augmentation within the framework of sharp liquid-solid interfaces. This significantly simplifies the implementation, particularly for reactions occurring in porous media with intricate geometric structures. Several benchmark tests were performed to validate the accuracy of this model, including a reaction-diffusion problem in a rectangular domain, a two-dimensional reaction and dissolution of a circular grain, as well as a three-dimensional calcite crystal dissolution in a micro-channel. All the obtained simulation results agree well with the reference solutions. In addition, a dissolution problem in a three-dimensional porous meida bulit with the sandpack is then investigated. Cases with different Peclet numbers (Pe) and Damkohler numbers (Da) were simulated, and five dissolution modes were obtained, which were finally summarized in a diagram of Pe and Da.

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Diffusion Hysteresis in Unsaturated Water Flow: A Microfluic study

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In unsaturated flow studies, water saturation is commonly used as the sole descriptor for macroscale flow models. However, this approach often results in hydraulic hysteresis in capillary pressure and relative permeability during drainage and imbibition processes. Furthermore, the effects of these behaviors on solute diffusion remain unclear. To address this knowledge gap, we conducted microfluidic experiments to investigate these hysteresis relationships. We firstly implemented drainage and imbibition processes in the micromodel to establish pore-scale water configurations. Subsequently,

we upscaled the capillary pressure and diffusion coefficients to the Representative-Elementary-Volume scale. Our results revealed that, at the same saturation levels, the unsaturated diffusion coefficients during drainage were at least 6.1% higher than during imbibition, indicating the presence of diffusion hysteresis. We observed that this hysteresis was influenced by capillary number and residual water saturation. An increase in the capillary number reduced diffusion hysteresis, similar to the capillary pressure hysteresis. While a decrease in residual saturation rose diffusion hysteresis. We also proposed a quadratic polynomial model that effectively predicts the diffusion coefficient by incorporating both saturation and capillary pressure. This research emphasizes the importance of historical changes in unsaturated water flow, which hold significant implications for modeling solute transport processes.

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Poster / 994

The role of biopolymer on the stability of Colloidal Gas Aphrons

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Numerous studies 1 have been conducted on using surfactant solutions for soil remediation, but their implementation has been limited by the high cost and consumption 2 of surfactant solutions. Moreover, CGA fluids have been shown to be more effective than surfactant solutions in terms of contaminants eliminated per gram of surfactant [3]. An innovative approach to address these challenges is the use of colloidal gas aphrons (CGA) fluid, which aims to reduce the cost of the operation compared to traditional surfactant-based soil remediation. The first investigation into the stability of CGA fluid for soil remediation was done in 1994, where volume fraction and bubble size distribution of microbubbles in sample solutions were measured over time [4].
CGAs were first introduced by Sebba in the 1970s [5] as a new form of dispersion characterized by gas bubbles dispersed in a continuous liquid phase. Colloidal gas aphrons are stabilized by a viscous water layer and surfactant shells, creating a microbubble system [6]. However, CGA-based fluids must remain stable to prevent the destruction of bubbles when injecting them into porous media for soil remediation purposes. This ensures their effectiveness and benefits [7]. The size of the bubbles, which is determined by the surfactant, is one of the most critical factors influencing CGA stability. Although previous studies have examined the use of CGA for oil industry applications such as drilling fluid or injection into depleted reservoirs, its application for soil remediation studies is not

yet clear [8]. Furthermore, the impact of additional stabilizers and thickeners, such as polymers, has not been thoroughly investigated. Therefore, it is crucial to investigate how quantitative parameters like surfactant and polymer concentrations at high levels affect the stability of CGA.
The primary objective of this research study is to investigate the impact of a particular biopolymer and anionic surfactant at high concentrations on the stability of CGA using image analysis based on microscope images at varying concentrations.
The stability of CGA dispersion was analyzed by quantifying the bubble diameters using microscopic observation. Zeiss CCD camera was placed on a microscope slide to capture images of CGA fluid samples. Our study incorporated varying concentrations of xanthan gum polymer (ranging from 1000 to 10,000 ppm) and sodium dodecyl sulfate surfactant (ranging from 1 to 10 CMC). Subsequently, ImageJ software was used to analyze the images and determine the bubble size distribution (BSD) over time. Our evaluation involved determining the BSD at intervals of 0 to 10 minutes over 60 minutes.
The effects of SDS surfactant concentrations and XG polymer concentrations on BSD CGA were investigated experimentally using optical microscopy. The findings demonstrated that while the BSD of CGAs decreased at first with increasing XG polymer concentration, it eventually increased slowly. On the other hand, the diameter of CGAs increased with the concentration of SDS surfactant. Furthermore, the greater viscosity of the base fluid due to higher polymer content led to reduced air penetration and smaller bubbles, resulting in slow gas diffusion and a lower gas fraction.

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A Novel Approach for Advancing Lithology Classification Through Machine Learning and Deep Learning Models

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Manual interpretation of geophysical logging data can be a tedious and time consuming task in the case of the non-linear behavior of well-logging signals. In this study, we introduced three novel algorithms including GrowNet, Deep-Insight and blender in the classification of rock facies. To compare the performance of these models, we used algorithms such as XGBoost, Random Forest and Support Vector Machine. The data employed is from the South and North Viking Graben, comprising twelve lithological rock facies. Deep-insight was used to convert tabular data into images and these generated images were employed as inputs for a convolutional neural network. It demonstrated better performance in lithology classification compared to traditional models such as Decision Tree and Logistic Regression. The GrowNet and blender models for lithology classification successfully increased the penalty score and accuracy compared to the FORCE2020 competition. This study highlights the value of a hybrid approach, integrating the SMOTE and NearMiss algorithms in order to balance the data. Addressing missing data is crucial for dependable analysis; employing regression models, rather than simplistic techniques such as mean imputation, enhances accuracy. Additionally, knowledge-based feature augmentation techniques are selectively applied based on the availability of relevant features, thereby enhancing the effectiveness of the overall model learning process. To more efficiently evaluate and compare the performance of the models in a multi-class classification, we introduced the class prediction error plot instead of using confusion matrix.

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Pore-scale experimental investigation of low-salinity waterflooding for enhanced oil recovery

Author: Chunyu Tong[1]

Co-authors: Jun Yao ; Yongfei Yang

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Low-salinity waterflooding (LSWF) is a promising enhanced oil recovery method that has shown exciting results in various experiments conducted at different scales. With the development of imaging technologies, micro-CT is also employed to investigate LSWF and the synergistic effects of low-salinity brine and polymer. Micro-CT enables the observation of fluid behaviors and the explanation of mechanisms, providing a comprehensive understanding of the pore-scale displacement process during LSWF.

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Poster / 999

Experimental and simulation study on enhanced oil recovery of sandstone reservoir in high water cut stage

Author: Tao Wang[1]

Co-authors: Haiyang Yu [1]; Fei Wang [2]; Xuchen Zhu [2]; Jie Hu [2]; Xinyu Lin [2]; Yuqing Zhu [3]

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Sandstone reservoir has good porosity and permeability, which is one of the main oil and gas reservoirs and the focus of oil and gas resources development. Water injec-tion development is the main way of sandstone reservoir development, but with the continuous increase of development time, the water cut of the reservoir is increasing, a large number of reservoirs are in the high water cut stage, and the efficiency of water injection development is decreasing. Therefore, it is very important to master the formation and distribution characteristics of remaining oil in high water cut reser-voir and its producing mechanism for the further development. In this paper, the remaining oil in the core pores of the high water cut stage is visualized on the micron scale by CT scanning, and the oil-water flow simulation and the remaining oil produc-tion simulation are carried out based on the digital core technology. The results show that the distribution of remaining oil in high permeability reservoirs is less but more dispersed, and the remaining oil in low permeability cores is more connected. The remaining oil content of high viscosity crude oil reservoir is high. By reducing the in-terfacial tension, the water phase can invade more pores to achieve the effect of remaining oil production. This study is helpful to guide the high water cut sandstone reservoir to take measures to further improve the recovery rate and realize the further development of the reservoir.

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Poster / 1000

Pore-scale Modeling of Dynamic CO2 Dissolution in Natural Porous Media with different Wettability

Authors: Jinlei Wang[None]; Yongfei Yang[1]

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In oil-gas-water three-phase systems, CO2 can be distributed either as a non-wetting phase, or as an intermediate-wetting phase. The morphology and distribu-tion of CO2 clusters under different wetting sequences are different, which has a complex influence on CO2 dissolution process. Based on phase distribution ob-tained from three-phase flow experiment, we constructed the physical models of initial CO2 phase distribution, subsequently simulated the CO2 dissolution pro-cess when CO2 is non-wetting phase and intermediate-wetting based on the VOF framework and CST method. The dynamic evolution of CO2 clusters and dis-solved CO2 distribution during dissolution process was tracked. The effect of wettability on CO2 dissolution trapping in three-phase systems was revealed. The characteristic parameters of CO2 dissolution process were also analyzed quantita-tively. Our results showed that CO2 clusters exhibited different dissolution states under different wetting conditions in three-phase systems. When CO2 serves as intermediate-wetting phase, the initial phase distribution is more dispersed, and the size of CO2 clusters is smaller, the CO2 saturation decreases more within the same time period, indicating that CO2 has a higher dissolution ability. The initial CO2 saturation determines the final CO2 concentration in the other phase. Disso-lution caused the originally connected large CO2 clusters to decompose into mul-tiple small clusters. When CO2 serves as intermediate -wetting phase, the mass of dissolved CO2 is higher, and thus the dissolution ability is higher.

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Poster / 1001

A fully implicit single-phase multi-component phase transition pore network model based on automatic differentiation and GPU

acceleration

Authors: Chaozhong Qin[1]; JIanqi Rong[1]

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The complex phase behavior of hydrocarbon mixtures is encountered in miscible flooding in the oil-saturated reservoir and liquid dropout in gas-condensate reservoir. In pore-network models, phase equilibrium calculations (Michelsen, 1982) have been coupled with convective-diffusion equations to evaluate the influence of hydrocarbon phase behaviors to flow and transport at given hydrocarbon mole compositions and temperature, as reported by Chen et al. (2020) and Santos, M.P.P.C. et al. (2020) where a fully implicit Euler method is implemented to get the set of non-linear algebraic equations at each time step solved by Newton's method.

The number of convective-diffusion equations varies with pseudo-components number, which brings great inconvenience to the analytical programming of Jacobian matrix. In this work, the reverse derivation technique based on the chain derivation rule (Baydin et al., 2017) is applied to evaluate Jacobian matrix using a open source C++ library named fadbad++ and the program is comparable in time to the analytical programming of Jacobian matrix.

In addition, the GPU parallelization is promising to the numerical studies of multi-component flow and transport with computationally intensive nature. In our test, a graphic card RTX 3060 with 12GB memory together with CUDA library is used to speed up the steady-state and transient simulation process. The program is compared with the one running on a CPU i5-12400F with the Eigen mathematical library. The comparison results show that the acceleration rate can be about 5 times in the single-phase dynamic simulation with a pore network of 8000 pore elements, and about 10 times in the single-phase steady-state simulation with 2 million pore elements.

The coupled model is used for gas-condensate reservoir simulation to investigate the effect of droplets on gas production processes. In future work, a more efficient coupling way will be explored (Collins et al., 1992), and the existing model will be advanced to two-phase flow simulation (An et al., 2023).

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Poster / 1002

Archaea community in gas hydrate-bearing sediments in the South China Sea

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The South China Sea, endowed with abundant natural gas hydrate resources, presents exceptional conditions for gas hydrate formation and exploration prospects. Gas hydrate-bearing sediments are characterized by methane saturation in pore waters, fostering rich and distinctive microbial ecosystems. These microorganisms play crucial roles in methane production, consumption, and global carbon cycling. This study focuses on 117 sediment samples from 11 sites across the Qiongdongnan Basin, Shenhu area, and Xisha Trough of the South China Sea , employing high-throughput MiSeq sequencing of the 16S rRNA gene to investigate the archaeal community structures and diversity. Our findings highlight significant microbial diversity variance across samples from the three geographic regions, with distinct differences noted between samples from the Qiongdongnan Basin and Shenhu area. The archaeal population is dominated by Halobacterota, Hadarchaeota, Lokiarchaeota, Euryarchaeota, and Woesearchaeota. Notably, methane-metabolizing taxa are prevalent, with a significant abundance of methanogenic archaea over anaerobic methane-oxidizing archaea (ANME). Additionally, the structure of methane-metabolizing groups varies significantly across the three regions, with ANME predominantly identified in the Qiongdongnan Basin. Methanogens show differing dominance in the Shenhu area compared to the Qiongdongnan Basin, and only a few methanogenic groups were observed in the Xisha Trough samples. This study provides the characteristics of archaeal community diversity within sediment cores from gas hydrate-bearing sediments in the South China Sea, contributing to our understanding of microbial group characteristics in these regions. Understanding these microbial populations and their functions is crucial for the comprehension of the biogeochemical processes involved in the formation of natural gas hydrates in the South China Sea.

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A variational hydraulic fracturing model for simulating the hydraulic fracture propagation in fracture-caved porous media

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The fracture-caved porous media contains numerous irregular natural fractures and caves, leading to multiscale pore structures. The geometry of these pore structures can impact the mechanical characteristics of the porous media, and also significantly affect the hydraulic fracture propagation path. This study presents an innovative hydraulic fracturing model designed to simulate the fracture propagation within fracture-caved poroelastic media, leveraging the capabilities of the phase-field method. Initially, the fracture-cave-reservoir flow governing equations are established through coupling generalized Reynolds flow in the fracture domain, Darcy flow in the reservoir domain and free flow in the cave domain. Biot poroelasticity theory and fracture width serve as the links for hydro-mechanical coupling. To address sharp fractures and cave edges, a smooth phase-field method is introduced. The fully coupled model is solved using a staggered scheme, which independently addresses the pressure and displacement fields in the inner cycle, and then addresses the phase-field in the outer cycle. In contrast to prior research, our model eliminates the need for supplementary enrichment functions to characterize natural fractures and caves. It can naturally detect and simulate the behavior of hydraulic fracture propagation in the presence of natural caves. This alleviates the complex calculations of stress intensity factors as hydraulic fracture nears caves. The efficacy of the proposed model in addressing two-dimensional scenarios is thoroughly demonstrated. Subsequently, the model is expanded to encompass three-dimensional scenarios and multiple cave instances.

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Probabilistic and statistical modeling of inflow into a well after hydraulic fracturing

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Hydraulic fracturing technology improves the productivity and economic benefits of an oil and gas wells, but there are many factors affecting productivity and it is difficult to evaluate productivity. Information amount theory (IAT) method is using to evaluate and analyze the factors affecting production capacity after hydraulic fracturing of the wells. Based on the statistics simulation of productivity influencing factors of wells fractured in carbonates deposits of Perm region fields, the information amount theory method is used to analyze geological and technological parameters. In order to create a multi-variable model to estimate the oil production post-fracking increase, the well sample is divided into two roughly parts. The productivity increases with increasing the oil production rate after fracking and the fracture width.
A multiple linear regression model was constructed using input features fracture length, fracture width, Propant Height and other parameters. The developed model provided a R2 value 0.8792. The result indicated that the model was able to explain 63.7% of the oil production variance in the study area.
The reported study was partially supported by the Government of Perm Krai, research project No. СЭД-26-08-08-32 from 25.01.2024

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1005

A Review of the Application of Metaverse Technology in Petroleum Engineering

Authors: Jing Lu[None]; 聂庆[None]

Co-author: Erlong Yang

Corresponding Author: 871789003@qq.com

In the context of accelerating digital transformation in the energy industry, the metaverse, as an emerging concept of virtual world, is becoming a crucial foundation for the new revolution in oil and gas fields. Metaverse technology offers novel digital solutions for oil and gas fields, driving the development of smart oilfields and enabling the industry to explore and produce oil and gas more intelligently and efficiently. This paper aims to delve into how the metaverse, as a digital space integrating virtual and real worlds, is applied in the domain of oil and gas fields to address challenges in exploration, production, and other processes. It explores the current status and prospects of metaverse technology application in oil and gas fields, thoroughly analyzes its application in oil and gas exploration, discusses the feasibility and advantages of metaverse services and integration with oil and gas fields, and summarizes existing challenges.

Keywords: oil and gas exploration, smart oilfield, metaverse

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MS05 / **1006**

Pore-Scale Modeling MICP Process and Investigation of the Effect of Pore Structures on Calcite Distribution

Authors: Dianlei Feng[None]; yajie chu[None]; Leiyu Feng[None]; Lingxiang Wang[None]

Corresponding Author: cyjxs2018@126.com

Abstract: The microbially induced calcite precipitation (MICP) technique holds promising applications in groundwater remediation, gas storage, soil improvement, and rock fracture sealing. In this study, a two-dimensional pore-scale numerical model is developed to simulate the coupled flow, reactive mass transport processes, and precipitation processes in MICP. In the presented model, the lattice Boltzmann method (LBM) and finite element method (FEM) are employed to solve the incompressible Navier-Stokes equations and the advection-diffusion-reaction (ADR) equation, respectively. The presented model considers the processes of bacterial transport and attachment, ureolysis, and the bacterial and calcite detachment induced by the shear effects of the flow. With the presented model, multiple field profiles including the flow field, concentration field, and the calcite distribution can be obtained in the pore space. The presented numerical model is validated based on the experimental data from the literature. To investigate the effect of heterogeneous pore structures on calcite distribution, different scenarios are carried out. The simulation results demonstrate that the pore structures with large pore throats result in more calcite accumulation. For heterogeneous pore structures with upper or lower distribution, the calcite distribution is dominated by the flow direction. Moreover, the quantitative results are presented in the evolution curves of calcite proportion, and the trend of evolution curves in different areas can reflect the homogeneity of the calcite distribution. The distribution of the evolution curves in various areas is aggregated, indicating a uniform calcite distribution.

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1008

RESEARCH AND APPLICATION OF QUANTITATIVE CHARACTERIZATION METHODS FOR RESERVOIRS UNDER THE SHIELDING OF IGNEOUS ROCKS

Author: Dong Ma[None]

Co-authors: Chao Li [1]; Hanqing Zhao [1]; Ming Yang [1]; Jianli Yan [1]

[1] *(Tianjin BRANCH of CNOOC)*

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Bozhong A Oilfield is the first sandstone reservoir discovered and put into development in an igneous rock development area in Bohai. The main oil bearing layer in the oilfield is the Paleogene, which is affected by igneous rocks and has strong reservoir heterogeneity. The development situation of production wells at the edge of igneous rocks is poor, and it is affected by the high-yield strategy of offshore sparse wells. The well spacing is large, and quantitative characterization of reservoirs is difficult. On the basis of summarizing the development characteristics of igneous rocks, this article comprehensively describes the micro pore structure characteristics of sandstone reservoirs in different regions of the oilfield through various analysis and testing methods such as petrography, high-pressure mercury injection, and nuclear magnetic resonance. Based on this, the quantitative transformation of sandstone reservoirs by igneous rocks is carried out based on the thermal solid coupling effect. According to the distribution pattern of igneous rocks and the mutual positional relationship between reservoirs, Extracting a model of the contact relationship between igneous rocks and reservoirs, considering the influence of parameters such as thermal conductivity, reservoir skeleton deformation, and stress sensitivity, a mathematical model for quantitatively characterizing the permeability of sandstone reservoirs under the influence of igneous rocks was established. Finite element deformation was used to solve the problem, and a quantitative characterization diagram of the degree of volcanic activity on sandstone reservoirs was drawn. The research results indicate that the thermal baking effect of igneous rocks in Bohai A oilfield reduces the permeability of reservoirs around 100m of igneous rocks. The closer to the boundary of igneous rocks, the more severe the decrease in reservoir permeability. Based on the research results, the three-dimensional geological model has been updated, and the numerical simulation accuracy has been improved from 70% to 92%. This provides a reference for reservoir evaluation and development plan design in similar oil fields.

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1009

Effect of interfacial tension reduction agents on fluid flow and oil production in reservoirs with low permeability layers

Author: JACQUELINE NANGENDO[1]

Co-authors: Aifen Li [1]; Li Tianhao [1]; Hu Zhuocheng [1]; Fu Shuaishi [1]; Gloire Imani [1]; Guoqiang An [1]; Huapeng Jing [1]; 立圆董

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The application of interfacial intension reducers (surfactants) in oil recovery has been widely applied because of the ability to reduce the interfacial tension in immiscible displacement. They also can change the wettability of the porous media to more water-wet and emulsify the oil to displace it in the subsurface porous media. Using surfactants to improve the performance of steam-assisted gravity drainage (SAGD) has been an intriguing idea for decades. This has been attributed to the ability of surfactants to form emulsions with oil and reduce interfacial tension (IFT) of the oil-water system which allows more oil to drain out of the reservoir. According to earlier research, surfactants increase oil's relative permeability by decreasing the IFT, de-wetting the surface, and emulsifying oil droplets, which increases oil mobility and displacement. In addition, this phenomenon can reduce the capillary pressure and enhance spontaneous imbibition. Therefore, some surfactants may increase production in reservoirs with barrier layers if carefully selected. Surfactants reduce interfacial tension (IFT) in the oil-water system, making the barrier layer extremely water-wet. In this study, numerical simulation using CMG-STARS backed up by experimental studies has been conducted. Several selected surfactants have been used to investigate their ability to overcome the challenges and impedance of the barrier layer on steam chamber expansion and the flow of oil across them to production. The simultaneous injection strategy was employed in both experimental and simulation studies. The surfactant played a great role in overcoming the barrier layers' effect on steam chamber expansion, oil production, and production rates increasing the flow of steam and oil across the barrier layer. From the experimental and simulation studies, the project with surfactant co-injection produced more oil and had greater oil production as compared to the pure-SAGD projects for various barrier layer thicknesses of a given permeability. The ability of the surfactant to enhance steam chamber growth, oil production, and production rate was seen to decrease with increasing and decreasing barrier layer thickness and permeability respectively. The residual oil results also showed significant differences in residual oil saturation (unproduced oil) for a given reservoir thickness and permeability under the same operation parameters. The steam flow and oil drainage across the low permeability layer were significantly greater and therefore reduced the amount of unproduced oil by over 50% compared to the pure SAGD process. The oil recovery rate also increased by almost two-fold while the oil production rates were one and a half times higher than pure SAGD at any given production time.
Keywords: Surfactant-aided SAGD, Steam chamber growth, Improved SAGD, Chemical-SAGD, Chemical-aided, thermal oil recovery, low permeability layers

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MS13 / 1010

Theory of electrolyte solutions in a slit charged pore: Effects of structural interactions and specific adsorption of ions

Author: Victoria A. Vasileva[1]

Co-authors: Daria Mazur [2]; Yury A. Budkov [3]

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[2] *Laboratory of Computational Physics, HSE University,*

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The study of electrolyte solutions in confined geometries is crucial for developing energy storage devices and water purification systems. One challenge in this field is accurate modeling ion behavior while considering the interplay between ion-specific effects and electrostatic interactions. Although self-consistent field theory enables the simulation of ionic fluids, it overlooks several effects, such as short-range correlations of the ions. Recent research 1 incorporates into the grand thermodynamic potential of ionic fluid the short-range correlations of the ions and derives the mechanical equilibrium condition using the Noether's theorem formalism. In particular, the authors have derived the total stress tensor of ionic fluid taking into account electrostatic and steric interactions alongside the structural effects (short-range correlations).

In this work, we use the model developed by Blossey et al. 2, which takes into account both structural and steric interactions between ions. The structural interactions are described through a bilinear form of the gradients of the local ionic concentrations, while the steric interactions are modeled using the lattice gas approach.This framework allows for a phenomenological description of the molecular properties of ions, such as steric interactions due to their non-spherical shape, changes in configuration, and the influence of the solvent. Additionally, we investigate the specific interactions between ions and pore surfaces by incorporating external attractive forces.

Our main interest lies in analyzing how ionic concentration profiles and disjoining pressure are influenced by variations in pore size. Starting from the local mechanical equilibrium condition, we derive a general formula for the disjoining pressure.
Our findings [3] indicate that taking into account the structural interactions between ions leads to a pronounce minimum in the disjoining pressure curves at small pore widths. This minimum is attributed to the formation of electrical double layers on the electrically charged surfaces of the pores.In addition, our results indicate that the attractive interactions between ions and the pore walls contribute to the formation of this minimum and shift it to smaller pore sizes. These theoretical findings have practical implications for researchers in the field of electrochemical engineering for supercapacitors, particularly in applications involving porous electrodes filled with concentrated electrolytes and room temperature ionic liquids.

1 Brandyshev P. E., Budkov Y. A. Noether's second theorem and covariant field theory of mechanical stresses in inhomogeneous ionic liquids. The Journal of chemical physics. –2023.–T. 158. –No. 17.
2 Blossey R., Maggs A. C., Podgornik R.Structural interactions in ionic liquids linked to higher-order Poisson-Boltzmann equations. Physical Review E. –2017
[3] Victoria A. Vasileva, Daria A. Mazur, Yury A. Budkov. Theory of electrolyte solutions in a slit charged pore: Effects of structural interactions and specific adsorption of ions. Journal of Chemical Physics. 2023. Vol. 159. No. 2. Article 024709

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Poster / 1011

The Future of Core Analysis: Estimating of Effective Porosity via µCT & Transfer Learning

Author: Rail Kadyrov[1]

Co-authors: Evgeny Statsenko [1]; Thanh Hung Nguyen [1]

[1] *Kazan Federal University*

Corresponding Authors: thanhtu154@gmail.com, e.statsenko@yahoo.com, rail7777@gmail.com

Currently, µCT has emerged as a valuable tool for analyzing rock samples on a standard core plug scale. Typically utilized in Special Core Analysis (SCAL) as an assessment instrument before the filtration experiment, µCT serves to examine core samples and identify any potential defects, cracks, or heterogeneities that could influence flow behavior during the procedure. Despite the relatively low resolution of such µCT images, they contain valuable information on lithological features and reservoir properties. This study focuses on the development and validation of an integrated methodology that combines µCT scanning of core plugs with machine learning algorithms to predict effective porosity values. For this work, we created a dataset of microtomographic images for standard samples of various types of reservoir rocks and annotated all images based on experimentally determined values for the samples. Utilizing a transfer learning approach, we trained a ResNet50 model to predict effective porosity values for standard core plugs. The results demonstrated high validation scores for the obtained values. This approach can be used to optimize Standard Core Analysis (SCA) procedures, reducing the time and financial costs associated with hydrocarbon extraction procedures from core plugs.

Acknowledgments
This work was supported by the Ministry of Science and Higher Education of the Russian Federation under agreement No. 075-15-2022-299 within the framework of the development program for a world-class Research Center “Efficient development of the global liquid hydrocarbon reserves”.

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1012

Study of the influence of carbon sequestration in rocks on changes in reservoir characteristics

Authors: Hongwen Jing[1]; Mikhail Turbakov[2]

Co-authors: Evgenii Riabokon [2]; Evgenii Kozhevnikov [2]

[1] *China University of Mining and Technology*

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The issues of carbon sequestration in natural porous media have recently received increasing attention in the scientific community. Scientists have obtained laboratory results, and carbon sequestration projects are already being implemented in a number of countries (Norway, USA, the Netherlands and Australia). One of the priority and most logical directions for the development of carbon sequestration in Russia is the additional extraction of hydrocarbons from fields that are at a late stage of development. Most hydrocarbon fields in the Perm region are at the final stage of development and could potentially be targets for carbon sequestration and additional oil production. However, the influence of carbon on natural porous media (rocks) is poorly understood and requires both laboratory research and the subsequent development of mathematical models of the influence of carbon on the filtration and mechanical characteristics of the formation in the long term. For the predicted result of carbon sequestration in rocks, it is necessary to justify the modes of injection of carbon dioxide into reservoir layers and long-term storage modes under which gases are absorbed by the rock.
China is also interested in the development and implementation of carbon sequestration, since it, like Russia, is in the top five countries for carbon emissions per year and is looking for new solutions to improve the quality of atmospheric air in industrial regions, in particular, in the direction of using waste coal mines .
The results of the present studies contribute to the development of carbon sequestration in coal rocks.
The reported study was partially supported by the Government of Perm Krai, research project No. СЭД-26-08-08-26 from 23.01.2024.

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The reported study was partially supported by the Government of Perm Krai, research project No. СЭД-26-08-08-26 from 23.01.2024.

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MS03 / **1013**

Effective Characterization of Fractured Media with PEDL: A Deep Learning-Based Data Assimilation Approach

Author: Tongchao Nan[1]

Co-authors: Chunhui Lu [1]; Jiangjiang Zhang [1]; Jichun Wu [2]; Yifan Xie [1]

[1] *Hohai University*

[2] *Nanjing University*

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In various research fields such as hydrogeology, environmental science and energy engineering, geological formations with fractures are frequently encountered. Accurately characterizing these fractured media is of paramount importance when it comes to tasks that demand precise predictions of liquid flow and the transport of solute and energy within them. Since directly measuring fractured media poses inherent challenges, data assimilation (DA) techniques are typically employed to derive inverse estimates of media properties using observed state variables like hydraulic head, concentration, and temperature. Nonetheless, the considerable difficulties arising from the strong heterogeneity and non-Gaussian nature of fractured media have diminished the effectiveness of existing DA methods. In this study, we formulate a novel DA approach known as PEDL (parameter estimator with deep learning) that harnesses the capabilities of DL to capture nonlinear relationships and extract non-Gaussian features. To evaluate PEDL's performance, we conduct two numerical case studies with increasing complexity. Our results clearly demonstrate that PEDL outperforms three popular DA methods: ensemble smoother with multiple DA (ESMDA), iterative local updating ES (ILUES), and ES with DL-based update (ESDL). Sensitivity analyses confirm PEDL's validity and adaptability across various ensemble sizes and DL model architectures. Moreover, even in scenarios where structural difference exists between the accurate reference model and the simplified forecast model, PEDL adeptly identies the primary characteristics of fracture networks.

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MS17 / **1014**

Simulation study on the distribution of water - gas domains and two-phase seepage characteristics of coal based on the cavity throat network model

Author: Dong Zhou[1]

[1] *Taiyuan University of Technology*

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In order to investigate the influence of water gas domain distribution on the relative permeability of water and gas during the injection of hot water into coal, this paper establishes a two-dimensional pore cavity throat model based on fractal theory, and uses the water gas dynamic equilibrium equation as the judgment condition for seepage calculation. The water and gas balance control equation of the cavity throat network was derived, and the distribution law of the water gas domain during coal seam thermal injection and drainage gas production process was clarified. Finally, the relationship between water injection pressure, fractal dimension, temperature and relative permeability was obtained. In the study of constant temperature water injection process, it was found that as the injection pressure increases, the gas chamber is constantly occupied by water, the saturation of water continuously increases, and the relative permeability of water significantly increases. The injection pressure is positively correlated with the relative permeability of water. During the constant pressure heating and drainage process, the increase in free methane leads to an increase in gas pore pressure in the model, overcoming capillary forces to discharge water. The higher the temperature, the water chamber is occupied by the gas chamber, and the distribution of the gas domain is wider. When percolation occurs, the relative permeability of the gas increases sharply, which is positively correlated with temperature and conducive to the discharge of water.

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Poster / 1015

Anti-hydrate Surface Design for Utilization in CO2 Sequestration Processes

Authors: Rui Ma[1]; yuanhao chang[None]; BO WANG[1]; Fanhua Zeng[1]

[1] *University of Regina*

Corresponding Authors: wbg373@uregina.ca, fanhua.zeng@uregina.ca, microrean@outlook.com, 691720562@qq.com

The undesired CO2 hydrates formation in wellbores or pipelines often poses a significant risk to production safety. CO2 hydrates can develop during numerous processes, such as CO2 injection for geological or saltwater storage, production wells in CO2 flooding for enhanced oil recovery, and CO2 pipeline transportation. These hydrates form when gas-water two-phase conditions are met within the hydrate stability zone. Particularly during the transition of supercritical CO2 into the gas phase, the decrease in temperature promotes the hydrate formation. Once these hydrates accumulate on a large scale and form blockages, the bulk hydrates significantly compromise the safety and efficacy of CO2 storage or hydrocarbon production. To address the challenges posed by hydrates, an

effective alternative solution is to develop a new generation of passive anti-hydrate surfaces that can prevent hydrates from accumulating over time. These new surfaces can incorporate smart properties such as anti-hydrate nucleation on the surface initially and possess low hydrate adhesion strength if hydrate deposition inevitably occurs. Therefore, it is necessary to understand the fundamental interactions between CO2 hydrates and solid surfaces. To achieve this, the current study employs systematic atomistic modeling and large-scale molecular dynamics (MD) simulations to explore the underlying mechanisms and key factors influencing hydrate adhesion. The results indicate that the gas concentration in the vicinity of solid surfaces plays a crucial role in determining the structures of the hydrates intermediate layer formed on those surfaces. By increasing the gas content near solid surfaces, it becomes possible to weaken CO2 hydrate adhesion, enabling the automatic detachment of hydrates under the influence of shear flow. With a better understanding of these mechanisms, it is conceivable to develop more effective anti-hydrate strategies and enhance the safety and efficiency of CO2 utilization process.

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Poster / 1016

Pore-Scale Insights into Freshwater Displacement Dynamics in Brine-Saturated Berea Sandstone Using 4D Microtomography

Author: Rail Kadyrov[1]

Co-authors: Evgeny Statsenko [1]; Thanh Hung Nguyen [1]

[1] *Kazan Federal University*

Corresponding Authors: rail7777@gmail.com, e.statsenko@yahoo.com, thanhtu154@gmail.com

In recent years, oil and gas companies operating in regions with high-salinity reservoirs have shown a growing interest in the processes occurring at the pore scale during the displacement of brine with freshwater. This interest is driven by the potential for freshwater injection to alter the physicochemical properties of the rock-fluid system within the pore spaces of the reservoir, thereby improving oil recovery. Such alterations can lead to changes in surface tension between oil and water, enhancing the mobility of oil within the porous medium and consequently increasing its extraction. Additionally, the interaction between the fluid and the rock matrix can affect the wettability of the rock; a transition towards more hydrophilic conditions could facilitate the easier displacement of oil by water. This study employs 4D microtomography to experimentally investigate brine displacement by freshwater in Berea sandstone at the pore scale under reservoir conditions using an X-ray transparent Hassler core holder. The in-situ visualization allowed for the mapping of salt concentration distribution within the fluid during displacement, capturing the main front of concentration drop

within the pore space of the sample. These observations were corroborated by breakthrough moment determination based on the measurement of electrical resistance at the sample's output. The findings provide direct insights into fluid mixing in complex porous media, offering both data and validation for pore-scale process modeling.

Acknowledgements
This work was funded by the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities, project № FZSM-2023-0014.

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MS13 / 1017

Using fractal theory to study the influence of movable oil on the pore structure of different types of shale: A case study of the Fengcheng Formation shale in Well X of Mahu Sag, Junggar Basin, China

Author: Hong Zhang[1]

Co-author: Kouqi Liu [1]

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In order to investigate the influence of movable oil on the pore structure of various shale types, this study systematically selected 19 shale samples from Well X in the Mahu Sag of the Junggar Basin. Initially, X-ray diffraction (XRD) analysis was conducted to classify the shale samples. Subsequently, the geochemical properties and pore structures of the samples, both pre and post oil extraction, were comparatively analyzed through Total Organic Carbon (TOC) content measurement, rock pyrolysis, and nitrogen adsorption experiments. Additionally, fractal theory was employed to quantitatively describe the impact of movable oil on the pore structure of different shale types.
The findings reveal that siliceous shale exhibits a higher content of movable oil compared to calcareous shale. Following oil extraction, there was a notable increase in both specific surface area and pore volume across all shale samples, with a more pronounced variation observed in the pore structure of siliceous shale as opposed to calcareous shale. Calcareous shale predominantly displays H2-H3 type hysteresis loops, indicative of ink-bottle-shaped pores, suggesting a relatively uniform pore structure. Conversely, siliceous shale exhibits a diverse range of hysteresis loops, reflecting its complex pore structure. The fractal dimension of calcareous shale samples appears primarily influenced by pore structure, exhibiting no significant correlation with TOC content before or after oil extraction. Conversely, the change in fractal dimension of siliceous shale samples demonstrates no clear correlation with either TOC content or pore structure, suggesting that variations in fractal dimension may arise from the combined effects of TOC and pore structure.

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MS22 / 1018

Process modelling of selective laser melting: Effects of powder bed quality and surface tension model

Author: yuyao Zhang[None]

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Selective laser melting (SLM), an additive manufacturing (AM) technique utilised for metals, is attracting increasing interest in creating complex and high-quality components. Compared to the traditional welding of bulk materials, the powder bed melting process in SLM presents a more complex physical profile arising from the molten-material flow in the interparticle voids. This work employed a numerical method to explore the evolution of the interfaces between different phases and understand this complexity. The interface features influence the defects of SLM-produced parts, including pore formation, fatigue life, and mechanical strength. Computational fluid dynamics (CFD) and discrete element method (DEM) were used to reproduce the melting and layering process, respectively. Compared with the CFD-DEM coupling method, the sequential method ignores the motion of particles during the melting while overcoming the inherent limitations of mesh size in the coupling method. In a fully resolved fashion, this CFD model can use a smaller mesh and accurately simulate the interactions between the laser beam and powder bed with fine-size particles. The simulated results were validated by benchmark experiments using the Ti-6Al-4V (Ti64) powder. This validated work further investigates the influence of packing quality, laser power, and surface tension model on the evolution of interfaces, and provides an effective way to evaluate the effects of processing parameters.

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Poster / 1019

The investigation of shale dynamical spontaneous imbibition with hydration damage and its influence on mechanical property

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Shale gas development is relied on long horizontal drilling. But shale is typical formation that wellbore instability often occurs, restricting long horizontal drilling in shale reservoir. Hydration damage is a major trigger of borehole collapse in shale. During drilling process, spontaneous imbibition (SI) is one of main methods of water phase entering into shale. After this invasion, hydration between water and clay happens, forming damage effect. Currently, there are plenty of works about shale hydration mechanism, but research of connection between SI and hydration is rare. The understanding of shale hydration evolutionary law during SI is not deep enough, restricting the improvement of drilling quality in shale reservoir.
Therefore, in combination with SI test and rock mechanical test, based on damage mechanical theory, characteristics of shale SI and hydration damage evolutionary law during SI have been clarified. The dynamical model of shale SI has been established considering hydration damage. Also, constitutive model of shale hydration damage during SI has been built. The analysis of shale SI process and energy response law in loading have been conducted. Results indicate that shale has strong SI in earlier stage, and the imbibition gradually becomes stable at later stage. Due to the influence of hydration, driving forces of SI (capillary force and osmotic pressure) are both in dynamical process. Resistance of SI gradually declines due to hydration damage, which is beneficial for shale SI. Besides, compared to conventional model, dynamical model of SI is more consistent with test results, proving hydration is a major factor of shale SI. In addition, shale damage degree is consistent with degree of SI. During SI process, hydration crack starts to propagate, decreasing mechanical strength and leading to the change from brittleness to plasticity. With increasing imbibition time and hydration degree, total energy, elastic energy and dissipated energy all show decline, indicating the decreasing mechanical stability. Outcomes improve the understanding of shale mechanical behavior, offering theoretical support for high efficiency and safety of long horizontal drilling technique in shale gas reservoir

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2 Fanhui Z, Zhang Q, Jianchun G U O, et al. Mechanisms of shale hydration and water block removal[J]. Petroleum Exploration and Development, 2021, 48(3): 752-761.

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Poster / 1020

Machine-Learning-Based Robust Optimization of Brine Extraction Well Placement in CCS Projects Using Fast Marching Method

Author: Hyunjee Yoon[None]

Co-authors: Hoonyoung Jeong [1]; Yeongju Kim

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In carbon sequestration projects, ensuring the safe management of reservoir pressure is essential for long-term security. The injection of CO2 can lead to pressure build-up, risking safety issues like caprock damage, induced seismicity, and potential leaks. While brine extraction offers a practical solution to mitigate those safety issues, it is crucial to optimize the location of the brine extraction well, especially in heterogeneous reservoirs.

Optimizing the brine extraction well location is computationally expensive, requiring numerous simulation runs to identify the most effective configuration. To perform robust optimization, which employs multiple reservoir models representing reservoir uncertainties, the computational complexity further increases.

In this study, we propose a machine-learning-based surrogate model that accurately predicts the effectiveness of the input well location with low computational cost. The proposed model incorporates the fast-marching method (FMM) to calculate the hydraulic connectivity and convolutional neural network (CNN) to extract the features of the connectivity map and predict the net present value (NPV). NPV is used as an objective function that represents the effectiveness of a brine extraction well. We applied this model to a CO2 injection site in the Pohang basin, Korea. Our model showed strong predictive performance, significantly reducing the computational costs by utilizing only 5% of the total location candidates.

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Poster / 1021

Novel Learning-based Pattern-Data-Driven Forecast Approach for Predicting Future Well Responses

Author: Yeongju Kim[None]

Co-authors: Bo Ren [1]; Hoonyoung Jeong [2]

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Accurately predicting future well response is crucial for making investment decisions in developing subsurface reservoir resources. Future well responses have been forecasted using history-matching methods, but traditional history-matching methods often incur high computational costs in calibration steps and have difficulties in maintaining geological constraints. Recently, data-driven forecast methods like data-space inversion (DSI) and learning-based data-driven forecast approach (LDFA) have been introduced to mitigate the computation cost and geological constraint issues of history-matching methods. However, DSI and LDFA have extrapolation, conditioning, and prediction variance issues. In this study, we propose two simple approaches, a learning-based pattern-data-driven forecast approach (LPFA) and an ensemble conditioning step (ECS), to resolve the issues associated with DSI and LDFA. For the extrapolation issue, LPFA provides accurate predictions by scaling prior data using observed data, even when the observed data are outside the prior data range. ECS resolves the conditioning and variance issues of LDFA and LPFA by selecting the predictions of ensemble learning that honor the observed data. The prediction performances of DSI, LDFA, LPFA, and ECS are compared using two well-known benchmark models (Brugge and Olympus models). All the forecast approaches showed reliable performance in predicting future well responses, achieving an average median relative error of 2~3% under a 2% noise level of the observed data. However, LPFA was the only approach that provided the most accurate predictions for future well responses when the prior data did not contain data close to the observed data. ECS improved the prediction performances of LDFA and LPFA in both the Brugge and Olympus models as it selects only the predictions from multiple learning models honoring the observed data.

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Poster / 1022

Assessment of CO2 Storage Capacities in Saline Aquifers Using Material Balance Equations

Authors: Sangkeon Park[1]; Hyunmin Oh[2]; Hyunjee Yoon[1]; Yeongju Kim[1]; Byungin Choi[3]; Wenyue Sun[4]; Hoonyoung Jeong[1]

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Estimation the capacities for CO2 storage plays a pivotal role in carbon capture and storage (CCS) projects. The material balance equation (MBE) approach, commonly applied in this domain, provides direct estimations of CO2 storage potential. Traditional MBE techniques, however, often compute the original fluid in-place volume via volumetric assessments without subsequent validation, posing challenges to estimation accuracy. Recognizing the impact of precise original fluid in-place volume calculations reflective of the reservoir's pore volume on storage capacity, our research introduces an enhanced MBE methodology. We evaluated the effectiveness of our enhanced MBE method through comparisons with a commercial reservoir simulator, applying it to both a constructed synthetic aquifer scenario and the Sleipner field model. The application to the synthetic aquifer scenario resulted in a notably precise CO2 storage capacity estimate, with a relative error of just 2.085%, based on data from a single year of injection. This high level of accuracy was similarly observed in the Sleipner field application, where the method achieved a relative error of 1.6873%. Our developed MBE method further demonstrates its reliability in accurately forecasting CO2 storage capacities across a range of conditions, including variations in grid sizes, rock properties, injection rates, operational strategies, and geological heterogeneity.

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1023

Searching Sweet Spots by Using Gradient Boosting Decision Trees and Generative Adversarial Networks

Author: Jorge Saldana[None]

Corresponding Author: jorgesaldana@gmail.com

Objective/scope

In the realm of searching for oil and gas accurately pinpointing 'sweet spots' —or regions, with resources and ideal drilling conditions—remains a crucial puzzle. This research presents a method that combines Gradient Boosting Decision Trees (GBDT) and Generative Adversarial Networks (GANs) to transform the identification of spots, in unconventional reservoirs. By leveraging the capabilities

of GBDT and the data generation skills of GANs the study aims to improve the accuracy and efficiency of exploration activities leading to more successful drilling operations and optimized resource extraction.

Methods

The methodology focuses on an approach; Initially, GBDT models undergo training using a range of geological, geophysical, and petrophysical data to forecast reservoir characteristics that signify favorable locations. These models leverage their capability to navigate linear connections, within multidimensional data providing in-depth forecasts on reservoir quality and potential output. Subsequently, GANs are utilized to create data in scenarios where authentic data may be limited or incomplete enhancing the reliability and precision of the models. This innovative blend enables an examination of subsurface data pinpointing locations, with exceptional precision.

Results

The combination of using both GBDT models and GANs has led to outcomes; The GBDT models, which have an understanding of reservoir data greatly improve the accuracy of predicting optimal drilling locations while the GANs enhance the dataset effectively ensuring that the models are well trained even when data is scarce. This collaboration not only increases the success rate of exploration endeavors by identifying drilling spots but also optimizes resource allocation thereby reducing both environmental impact and financial risks associated with exploration activities. Moreover implementing these AI methods, for identifying drilling locations has resulted in significant enhancements in operational efficiency and notable cost savings, in exploration and development processes.

Novelty

The innovative application of GBDT and GANs, in this study to pinpoint locations marks a breakthrough in the realm of oil and gas exploration. Combining the capabilities of machine learning with the abilities of generative modeling it establishes a fresh benchmark, for precision and productivity in the sector with the potential to transform exploration tactics and bolster the eco-friendliness of hydrocarbon extraction practices.

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1024

Application of Machine Learning Techniques for Rate of Penetration Prediction

Author: Jorge Saldana[None]

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Objective/scope

The emerging area of drilling optimization has increasingly acknowledged the role of predicting Rate of Penetration (ROP) in improving operational efficiency and cutting costs, within the oil and gas sector. This research project aims to utilize machine learning (ML) techniques to forecast ROP with precision by analyzing drilling data and current operational variables. By incorporating ML algorithms into the ROP prediction process the study intends to develop a forecasting tool that enhances drilling strategies streamlines drilling activities and notably reduces both time and expenses associated with drilling projects.

Methods

Our method involves taking an approach using a range of data that includes geological features drilling methods and operational details to teach and confirm various machine learning models, like decision trees, neural networks, and ensemble methods. These models are created to understand the linear connections, between different factors that influence ROP. The training process is carefully planned to make sure the models are accurate and can be applied in drilling settings. One important aspect of our method is using feature engineering and selection techniques to find the variables improving how well the model works and how easily it can be understood. Additionally, we carry out cross-validation. Adjust hyperparameters to improve model accuracy and avoid overfitting.

Results

The use of machine learning techniques, in predicting ROP has shown outcomes proving its capability to forecast ROP accurately and reliably. These ML models have surpassed methods for predicting ROP providing insights into the drilling process and allowing for proactive adjustments to drilling parameters for optimal real-time ROP. This results in drilling procedures reducing unproductive time and leading to significant cost savings. Notably the research also emphasizes how adaptable ML models are to settings and drilling conditions showcasing their versatility as a valuable tool for optimizing drilling operations. The practical implications of these discoveries are profound indicating that ML-driven ROP prediction could become an element in drilling optimization strategies. This would enhance decision-making processes and operational excellence, within the oil and gas industry.

Novelty

The study's uniqueness lies in its use of machine learning methods to accurately forecast the Rate of Penetration (ROP) in drilling activities, an aspect, of operational effectiveness in the oil and gas sector. In contrast to ROP prediction techniques, this study employs a range of ML algorithms along with sophisticated feature engineering and selection procedures to reveal the complex nonlinear connections between various drilling parameters and ROP. This strategy not only outperforms the precision of standard models but also introduces a level of flexibility and real-time relevance that was previously unachievable representing a significant advancement, in drilling optimization technology.

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MS03 / **1025**

Thermo-hydraulic-Mechanical Modeling Studies of Cryogenic Effects in the Near-wellbore Region of Geothermal Formations

Authors: Philip H. Winterfeld[1]; Bowen Yao[2]; Yu-Shu Wu[1]

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We developed a parallel thermo-hydraulic-mechanical (THM) model of fully coupled multiphase fluid and heat flow and geomechanics as well as associated fracturing processes in porous and fractured media to simulate cryogenic fracturing with liquid nitrogen in hot reservoirs. This included enhancing our THM simulator and developing a physical property module for nitrogen-water systems and formulating fracture initiation and extension criteria.

We used cryogenic fracturing experiments on small concrete blocks to verify the simulator modifications. Then, we simulated two field cases, one with an injector-producer pair with cryogenic fracturing that enhanced the permeability in a vertical plane around the wellbore and extending in the direction of the producer. The second case was cryogenic fracturing and cooling of the near-wellbore region in a shallow, heated reservoir. The induced fractures were horizontal but their lengths were non-uniform due to the pressure and temperature gradients.

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MS06-A / **1026**

Effects of particle density and pore fluid on granular flow in a rotating drum

Author: Yu Chen[1]

Co-authors: Si Suo [2]; Yixiang Gan [1]

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Effects of particle density and pore fluid on granular flow in a rotating drum
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The understanding of granular flow is of importance in many practical applications. This study employs both experimental and numerical analyses of dry and submerged granular media in a rotating drum, with a range of particle density. A continuum approach based on the two-phase flow and \mu(I) rheology is adopted, with all material parameters identified from experimental measurements. The accuracy of our model is evidenced by its ability to closely replicate experimental observations, particularly in the rolling and cascading stages. We specifically examined the dynamic angle of repose, flow region depth, and pore pressure behaviour within the granular region. The roles of particle density and pore fluid are demonstrated in distinct granular flow characteristics. We examine the solid pressure and fluid pressure distribution across the different cases in the submerged conditions. A significant advancement of our study is the normalisation of fluid pressure, which is achieved through a function of the Reynolds number, the contrasts in particle and fluid density. The unified correlation aligns with the principles of the Kozeny-Carman model. This work offers an effective numerical approach for design and optimisation of industrial processes involving granular flow.
Key words: granular flow; rotating drum; granular rheology; dynamic angle of repose; pore fluids

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1027

Utilizing Machine Learning for Surrogate Modeling: Analyzing Key Parameters in Underground Hydrogen Storage

Authors: Tanin Esfandi[1]; Yasin Noruzi[2]; Saeid Sadeghnejad[1]

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Renewable energy is attracting widespread interest worldwide as it emits minimal greenhouse gases, thereby aiding in the fight against climate change resulting from the use of fossil fuels 1. Hydrogen (H2) is suggested as a reliable energy carrier to address the fluctuations in energy supply faced by renewable energy sources 2. It can be stored for extended periods and harnessed to fulfill energy requirements [2-4]. Underground hydrogen storage (UHS) is crucial for integrating renewable energy and reducing carbon emissions. Its capacity for scalability, large-scale H2 storage, and grid stabilization are essential for sustainable energy transition. Utilizing geological formations enhances energy

security and maximizes excess renewable resource utilization, strengthening energy networks. Geological formations hold significant potential for long-term H2 storage [1, 4]. Among underground geological formations, depleted gas reservoirs have demonstrated effectiveness in storing natural gas underground [2, 5].
Physics-based reservoir simulations, although beneficial in assessing H2 injection and withdrawal processes, are also costly computationally, necessitating the simulation of every conceivable scenario [6]. Additionally, multiphase compositional reservoir simulations, particularly for three-dimensional field-scale scenarios, present obstacles to thoroughly analyzing and improving UHS systems 2. Utilizing machine learning techniques, surrogate models offer the potential to serve as an extra decision-making tool in the petroleum industry [7]. These methods are effective in lowering the computational expenses of simulations while still maintaining a reasonable level of accuracy [8-10]. Boosting algorithms, a subset of machine learning techniques, are particularly effective for this purpose. They iteratively enhance the performance of weak learners, enabling the model to learn complex patterns in the data [11]. Moreover, their versatility makes them suitable for the diverse datasets found in petroleum industry applications [12].
In this study, we developed a surrogate model using XGBoost, trained on datasets from a depleted gas field in the Middle East. These datasets included five crucial input parameters: cushion gas apparent molecular weight, formation pressure, formation dip angle, presence of fractures, and fracture density, which were derived from a commercial compositional simulator. The simulation of the UHS system unfolded in two stages, as mentioned below, and the objective was to evaluate the performance of the UHS system based on the H2 recovery factor.
I. Production from a single well was simulated over several years until reaching abandonment pressure levels, with abandonment pressures ranging from 1000 to 4000 psi.
II. The UHS process consists of two cycles, each comprising two phases, each lasting 6 months:
• An injection phase with a specified volume threshold.
• A withdrawal phase coinciding with high energy demand in the second 6 months of the year.
After careful testing and validation, the chosen boosting algorithm enabled the surrogate model to efficiently assess the effectiveness and recovery of H2 storage in underground reservoirs, achieving results multiple orders of magnitude faster than full-physics compositional reservoir simulation. These results can be considered representative since the study was conducted using actual data. Despite promising outcomes from the machine learning-based surrogate model, further research is needed to determine its potential as a complete replacement for assessing UHS system.

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Poster / 1028

RepoTREND: Software Tools for Robust Safety Analysis of Radioactive Waste Repositories

Author: Tatiana Reiche[None]

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RepoTREND 1, 2 is a novel simulator that has been designed to emulate the processes that occur within a radioactive waste repository in a variety of geological formations. It provides robust functionality to simulate the release and migration of contaminants from the near-field through the geosphere to the biosphere, while estimating their radiological impact on human health and the environment.

Designed with modularity in mind, RepoTREND consists of computational modules tailored to simulate the processes within each subsystem of a repository. The inherent heterogeneity of typical repository models poses significant challenges. In addition to fundamental processes such as two-phase contaminant transport, numerous specific effects (such as container corrosion or rock convergence) have to be considered in the simulation.

The structure of RepoTREND has been designed to meet a number of challenges. These include the flexible selection of models for different regions, the seamless combination of models during simulations and the easy integration of new models and effects. The RepoTREND code is a framework for the solution of a general nonlinear system of equations. Different physics are implemented as models in library form.

Each model is defined by specific equations of state and routines for handling relevant effects, organised in libraries of equations and effects. This structure simplifies the integration of new equations and effects, and allows different models to be assigned to different grid blocks. The coupling of physical models is managed implicitly. This facilitates the solution of linear couplings between variables across grid blocks within the same matrix system.

This conceptual approach ensures ease of implementation for new effects. It also maintains flexibility, transparency and reusability as the code is extended and refined.

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2 https://www.grs.de/en/news/projects/repotrend-repository-safety-analysis

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Poster / 1029

Droplet motion in flexible channels: Effects of opening angle and wettability

Author: Haiyi Zhong[None]

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Passive and directional droplet transport has gained significant interest due to their potential applications, e.g., self-cleaning surfaces and atmospheric water harvesting. One novel mechanism, known as *bendotaxis*, involves droplets spontaneously deforming an elastic channel via capillary pressure, thereby inducing droplet motion. However, current studies have primarily focused on parallel channels, neglecting the potential influence of channel geometry on droplet motion and transport efficiency. This study aims to investigate the combined effects of channel opening angle, structural flexibility, and surface wettability on droplet motion dynamics. We employ a comprehensive approach, combining macroscopic-scale experiments, numerical simulations, and a simplified mathematical model to explore different transport modes and their associated timescales. The current study offers insights into directional droplet transport phenomena, leading to potential technological advancements in various fields.

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Poster / 1030

Improving CO2 Sweep Efficiency in Carbonate Rock by Injecting Water-Saturated CO2

Author: Hang Yin[1]

Co-authors: Furqan Le-Hussain [2]; Jiachao Ge [3]; Patrick Tung [1]; YAMIN WANG [1]; Saira Saira [4]

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We present a comparison between water-saturated CO2 injection and CO2 injection into an Indiana limestone core. Micro computed tomography (micro-CT) imaging (Figure 1) and mercury intrusion capillary pressure (MICP) measurement (Figure 2) technologies were used to determine the pore size distribution. Results suggest that Indiana limestone consists of three pore sizes: large pores > 200 μm, medium pores in range 3-200 μm, and small pores < 3 μm. Pure CO2 or wsCO2 are injected into the core having crude oil and irreducible water at 70 ℃ and 12 MPa, representing near-miscible conditions.

wsCO2 injection yields 4.9% - 13.6% additional oil recovery (Figure 3d), and 19-36 times greater pressure difference across the core (Figure 3b). Our observations during wsCO2 injection suggest that water might be condensed into oil phase creating an emulsion (Figure 4). Emulsification leads to greater flow resistance therefore, the pressure difference increased. Results also suggest that pure CO2 could only displace crude oil from pores greater than 21 μm, while wsCO2 could entry into an order of magnitude smaller pores due to the 19-36 times higher ultimate pressure difference (Figure 5). The pore space vacated by additional oil recovery is occupied by CO2 yielding a 3% - 9% PV additional CO2 stored compared to pure CO2 injection (Figure 3f).

Keywords: CO2 injection; Water-saturated CO2 injection; Carbonate rock; CO2 storage.

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Poster / 1031

Experimental and Model Studies of Fluids in Micro-Nano Scales

Author: Fuquan Song[1]

Co-authors: Heying Ding [2]; Xiao Hu [3]; Jinbiao Yu [4]; Fei Gao [1]

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Since the beginning of the 21st century, fluid flow in micro-nano space has become a new research hotspot with the rapid development of micro-mechanical systems and bio- engineer-ing. Through quartz capillary and alumina channel, the flow characteristics of gas, water and oil were explored, and the flow characteristics of unconventional oil and gas reservoirs in micro-nano scale were studied. The corresponding nonlinear flow model, non-Newtonian fluid mechanics and neural network prediction model were established, which not only ex-plains the complex mechanism of fluid flow at micro-nano scale, but also provides theoretical support for application.
(1) Experimental studies of single-phase fluid at micro-nano scale: The gas flow be-havior in micro-nano channels was studied by means of experiments, and the gas flow under different conditions was analyzed. Through the flow experiments of deionized water and oil in nanochannels, it is found that the flow characteristics of water in nanochannels are differ-ent from those in traditional macroscales. The formulae of flow rate were derived for hydro-philic fluid, and were testified by experiments of deionized water flow in silica micro-channels. Finally, the non-Newtonian power-law fluid model of single-phase liquid was derived at the micro-nano scale.
(2) Experimental studies of two-phase flow at micro-nano scale: There are three stages in the change of gas flow rate when gas drives water at the micro-nano scale. In the first stage, there is a "pinning" effect of capillary pressure at the gas-liquid interface, and the flow rate increases slowly, which is about one order of magnitude lower than that of single-phase gas flow. In the second stage, a large amount of water in the nanoarray is displaced, finally the gas flow rate increases rapidly. A mathematical model of gas-liquid spontaneous imbibition was established. The validity of the model was verified by experiments, and the formula of the minimum resistance radius was derived.
(3) Application of neural network method in tight oil reservoirs：Based on the BP neural network method, the prediction model of non-Newtonian parameters in tight oil reser-voirs was established, and the average relative error is less than 5%. Based on Adam optimi-zation algorithm, a CNN-LSTM(Convolutional Neural Network-Long Short Term Memory) neural network model was established to predict the daily oil production of fractured hori-zontal wells in tight oil reservoirs. The model fully considers the heterogeneity characteris-tics of tight oil reservoirs, which effectively establishes the complex relationship between reservoir parameters and oil production.
Keywords: micro-nano channels, tight oil and gas reservoirs, Single phase and two phases flow, nonlinear flow.

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1032

compositionalIGFoam, a new Darcy-scale compositional solver

in OpenFOAM for CO2 / water interactions in CO2 storage processes in aquifers

Author: Ali Papi[1]

Co-authors: Amir Jahanbakhsh [1]; Mercedes M. Maroto-Valer [1]

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Evaporation and salt precipitation in Carbon Capture and Storage (CCS) processes in porous media requires further developments of the current tools and models. OpenFOAM, an open-source computational fluid dynamics (CFD) platform, offers a versatile environment for modelling complex fluid flow phenomena using its C++ object-oriented architecture. Various packages are available for simulating fluid flow in porous media using OpenFOAM. Despite the availability of these packages, the advancements in this area remain relatively under-developed. Further research efforts are needed to develop and refine current models, pushing the boundaries in this field. The OpenFOAM literature lacks a model that accounts for multicomponent interactions of multiphase flow systems (known as compositional modelling) at the Darcy scale. This work addresses this existing gap by introducing a new model in OpenFOAM aimed at the interaction between CO2 and H2O components in CO2 storage processes in aquifers; specifically, CO2 dissolution in water and water evaporation in CO2. The model, named compositionalIGFoam, extends the impesFoam solver of the porousMultiphaseFoam package 1 to incorporate a compositional solver that accounts for these phenomena.

In a Black Oil model such as impesFoam, the fluid phases are treated as two separate interfaces where the pressure and saturation equations are solved simultaneously. The word IMPES stands for Implicit Pressure Explicit Saturation where the pressure equation is solved implicitly at the current timestep, and the saturation equation is solved explicitly at the previous timestep to deal with the coupling of these two parameters. In a compositional model, the gas and liquid phases interact with each other through mass transfer. In this study, in order to solve for a compositional model, a two-phase (gas-liquid) binary component (CO2 –H2O) system is considered which means that two other species transport equations in the gas and liquid phases are added to the impesFoam solver and solved. Solving for one component would suffice as the other component can be calculated from that component. Additionally, the gas and liquid components are in equilibrium, and this is reflected in the form of Henry's law for the CO2 component, as the liquid will be a dilute solution. The model is further developed by considering an ideal behaviour.

Validation of the compositionalIGFoam solver was performed against existing examples, demonstrating its capability to reproduce the results while offering improvements in solution quality. Additionally, the model was applied to simulate gas injection into a water-filled core model, mimicking CO2 injection into aquifers and the results were compared against GEM CMG commercial compositional simulator. The results showed phenomenal agreement with GEM CMG model with only 1.8% and 0.4% error for both components, confirming the accuracy and reliability of the developed model.

In summary, this work contributes to advancing the state-of-the-art in porous media for modelling gas-liquid / fluid-rock interactions, species transport and phase equilibrium with OpenFOAM, offering a valuable tool for studying subsurface environments, particularly in the context of CCS and H2 storage processes, oil and gas reservoir engineering, and geothermal energies.

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Poster / 1034

Estimating sub-core permeability using multiple coreflooding experiments

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Coreflooding experiments are used regularly for reservoir rock characterization and have been developing in recent years. Investigation of sub-core phenomenon has been a topic of wide interest and estimating sub-core permeability distribution k(x,y,z) is important for that, and also for constructing accurate coreflooding models. This work presents a method for estimating permeability, combining data from multiple coreflooding experiments including different flowrates and fraction of injected fluids. Furthermore, the estimation accuracy considering a large number of physical parameters was studied. The method is shown to significantly improve the estimation accuracy in comparison to methods that incorporate data only from a single experiment which was studied in our previous work.

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1035

microfluidic to mimic red blood Cell flow in capillary

Author: marziyeh rahbar[1]

Co-authors: Nikolaos Karadimitriou ; Holger Steeb ; Jacques Huyghe [2]

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The study of microvascular function is vital for the understanding of numerous diseases: diabetes, heart failure, stroke, hypertension, vascular dementia, and erectile dysfunction. Several recent research on longitudinal capillary recruitment have found that capillary vessel haematocrit depends on the vasodilatory state of the arterioles. At rest, when the capillary pressure propulsion is at its minimum, vessel haematocrit is down to 15 %, suggesting a red blood cell (RBC) velocity three to five times higher than the plasma velocity in capillaries. This experimental result is at odds with all fluid mechanics models of capillary flow, indicating that understanding of RBC locomotion is failing at its most critical phase namely at the capillary level.

As pressure gradients generated by the heart typically propel the plasma and the RBCs jointly, and because the capillary pressure gradient is typically low at rest, the pressure gradient cannot be the driving force propelling the RBCs at the cost of plasma. What other forces are available to justify the observed unexplained behavior of RBCs in capillaries?

This study will address a new hypothesis, aiming at explaining the discrepancy between models and experimental observation, that the diffusion-osmosis and diffusiophoresis forces stemming from oxygen gradients at capillary entry are the most probable source of driving forces for propelling of the RBC at the cost of the plasma.

In this part of the project, an innovative microfluidic platform with oxygen gradient driving force is developed to emulate the capillary entry boundary conditions and to provide an insight into the use of this platform as a new promising tool in microvascular disease research for enhancing RBC propulsion in capillaries.

A microfluidic device is fabricated from Polydimethylsiloxane (PDMS). It consists of a central channel and two pairs of U-shaped channels on either side. RBCs flow through the central channel of 10-micron diameter. The left set of side channels emulated a pulmonary capillary. The reaction of hydrogen peroxide with sodium hypochlorite to generate oxygen is performed in left side channels. The supplied oxygen diffuses through the porous PDMS to the central channel and saturates RBCs with oxygen. The right set of perfused channels emulates a systemic capillary where oxygen is delivered to the environment. The U-shaped side channels on the right contain the oxygen scavenger absorbing oxygen emanating from the central channel. To quantify oxygen gradient within the central channel, an optical sensor is integrated to the microfluidic setup. The aim of the research is to draw out a paradigm for functionality of RBCs in capillary and offer an innovative microfluidic platform for research on microvascular disease.

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MS17 / 1036

Thermo-hydro-mechanical coupled zero-thickness interface finite elements: benchmarking and application

Author: wen luo[1]

Co-authors: Joaquin Liaudat [2]; Josselin Ouf [3]; Anne-Catherine Dieudonné [4]; Florian Amann [5]; Philip J. Vardon [4]

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Coupled thermo-hydro-mechanical (THM) processes play a key role in subsurface use, e.g. geothermal energy, CO2/H2 storage and geological repository. However, understanding these processes in porous media, in which natural fractures can be present and new fractures can be induced, is non-trivial task. The Cohesive Zone Model (CZM), a numerical technique in the framework of the Finite Element Method (FEM), is one of the possible choices in modelling fracture initiation and propagation due to its simple physical meaning and its mitigation of the need to calculate the stress singularity at the fracture tips that is commonly challenging in methods based on classical linear elastic fracture mechanics. In this work, we developed a THM coupled zero-thickness interface finite element employing CZM. It is developed to allow the simulation of longitudinal and transversal fluid/heat flow inside the fracture. The cubic law is used to simulate the fracture transmissivity as a function of its aperture, while an elasto-damage law is used to characterise the mechanical response of the discontinuity. The method is successfully verified against two analytical solutions: one of the coupled thermo-hydraulic response of a single fracture, and the KGD fracturing model that describes fracture propagation considering hydro-mechanical coupling. An example is then implemented to show how to simulate thermal fracturing without pre-defined fracture direction using the developed interface elements, and sensitivity analysis is performed against the injection rate and fracture energy.

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1037

Pore-scale Efficiency of Emulsion Flooding for the Removal of Organic Pollutants from Soils: Effect of Volume Fraction, Capillary Number and Wettability

Authors: Antonio Rodríguez de Castro[1]; Azita Ahmadi[2]; Aziz OMARI[3]; Shuxin WANG[4]

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In the field of environmental engineering, the remediation of nonaqueous phase liquids (NAPLs) present in polluted soils is challenging. Emulsions have proven to be efficient agents for physical in situ remediation 1. Pore-scale experiments using micromodels are often carried out to explore emulsion flow dynamics, characterize the movement of the liquid-liquid interface and visualize droplets retention [2, 3]. The objective of this study is to evaluate the effects of formulation and injection parameters on the efficiency of pollutant recovery via oil-in-water (O/W) emulsion flooding through experiments in microchips that mimic rock microstructures.

Used micromodels were either oil-wet or water-wet, with a pore width distribution ranging from 4 to 460 µm and constant depth of 20 µm. Their porosity and absolute permeability were respectively of 0.52, and 2.5 Darcy. Emulsions were formulated using rapeseed oil and tergitol NP35 as surfactant and the pollutant as well as used water were specifically dyed. The pollutant was brought to Sor after a classic waterflooding step and then emulsions with various characteristics were injected in the chip under observation of a microscope meanwhile recording the pressure drop. Acquired images were segmented and processed by means of ImageJ software.

First of all, we show that droplet's size distribution of all used O/W emulsions were not altered by their flooding through the microchips (Fig. 1a). However, on time scale of ten days, droplet size was seen to increase slightly (Fig 1b) due to ripening phenomenon. Fig. 2a showed typical raw images of the all successive steps of the process and Fig. 2b showed the post-treated corresponding ones that allow the computation of each phase's saturation. So, variation of pollutant saturation and pressure drop were followed during injection of at least 20 PV and this procedure was repeated for different volume fraction of droplets (Ø) of injected emulsions. As we can see the pollutant saturation reaches a limiting value that is lower for higher volume fraction (Fig. 3a vs Fig. 3b) and greater when the used chip is oil-wet as it would be expected (Fig. 3c). Moreover, the observed evolution of pressure drop displayed on these figures, is interpreted on basis of the considered flooding regime knowing values of capillary number, viscosity ratio and wettability and by taking into account the emulsion' s shear thinning character that is more pronounced for higher Ø values.
The images taken when the flooding process was over allow us to explain the mechanism of pollutant recovery and how it is enhanced by increasing emulsion's volume fraction (Fig. 3a1, Fig. 3b1). Besides, we can see clearly why the limiting oil saturation reached in case of oil wet chip was too high (Fig. 3c1).

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Poster / 1038

Two-Phase Flow Displacement Morphologies in Cohesive Granular Media

Author: Feihu KE[1]

[1] *The University of Hong Kong*

Corresponding Author: feihuke@connect.hku.hk

Multiphase flow in granular materials is intricate and subject to pattern formation resulting from the interplay between hydrodynamic and mechanical forces. While considerable effort has been devoted to studying systems with cohesionless grains, our understanding of the two-phase flow behavior through the cohesive counterpart held together by intergranular bonds is limited. Herein, we study the novel coupling between viscously unstable fluid-fluid displacement and bonded-grain deformation in a synthetic cohesive granular pack. We experimentally inject a low-viscosity fluid into a monolayer of cohesion-tuneable bonded glass beads that are initially saturated with a more-viscous fluid, with injection capillary numbers and cohesion levels varying among experiments. We map out a first-ever phase diagram showing displacement patterns transitioning from deformation-dominated fracturing with bond breakage to infiltration-dominated viscous fingering without grain motion as cohesion increases. Strikingly, we find that peak injection pressure exhibits a non-monotonic trend with increasing cohesiveness. The injection pressure reaches maximum when fracturing is favored against infiltration while begins to drop due to the regime transition irrespective of the increasing cohesion. Furthermore, we characterize the onset of fracturing via dimensional analysis, effectively capturing the transition based on the balance between viscous and cohesive forces. Our findings shed light on the multiphase flow behavior within cohesive materials which is fundamental in various subsurface technologies such as carbon geostorage, oil/gas recovery, and groundwater remediation.

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1039

Numerical investigation of flow stability and transition from Darcy to Darcy-Forchheimer regimes in a porous medium proxy

Author: Tairone Leao[1]

[1] *University of Brasilia*

Corresponding Author: tleao@unb.br

Darcy's law is part of a family of empirical linear laws in physics with fundamental importance for describing transport of heat, charge, matter, and energy. In its most general form, Darcy's law is a vector function with a second order tensor defining the permeability of the porous medium. For isotropic and homogeneous media, the permeability is a scalar constant and Darcy's law implies Laplace's equation when plugged into transport equations. In theory, Darcy's law should derive directly from more fundamental physical principles, in this case Stokes simplification of the Navier-Stokes equations for low inertia steady-state flow. In practice, rigorous derivations of Darcy's law from the Navier-Stokes equations are limited by the stochastic nature of porous media found in nature and by the difficulty in defining boundary conditions. The contact between the Darcy domain within the porous media and the free fluid domain, usually represented by Stokes'equation is an important theoretical constraint for understanding flow in real porous media, such as the contact between groundwater and surface-water in rivers, lakes and oceans and in flow from groundwater into wells, and in a range of natural and artificial filtration processes. This study investigates the effect of flow stability on the predictions of permeability from numerical simulations using OpenFOAM in a nonrandom porous medium proxy composed of nine cylinders of equal radius. The quasi-tridimensional domain represents flow in an array of spheres at the millimeter scale. The simulation investigates the transitions from free fluid into the porous domain and from the porous domain into free fluid. The effect of flow stability on permeability predictions is investigated using the Darcy and Darcy-Forchheimer equations and various forms of the Reynolds and the Forchheimer numbers are used to investigate the transitional regime. The effect of buffer zones for minimizing the effect of outlet jets is also investigated. Laminar and transitional regimes are investigated using direct numerical simulation (DNS) while flow on the transitional regime is also investigated using Reynolds-averaged Navier-Stokes equations (RANS) and Large Eddy Simulations (LES). Our results agree with the proposition that permeability is never constant even under creeping flow conditions. Under this proposition, the Darcy-Forchheimer equation is always the general case which reduces to Darcy's law when the inertia term tends to zero as flow velocity decreases. This also indicates the necessity of a better understanding of a generalized Darcy tensor which varies as a function of flow velocity. All forms of Reynolds and Forchheimer numbers tested were able to detect deviations from linearity caused by increasing inertia, however, the definition of the adequate form of the permeability coefficient for calculating some of the relevant dimensionless numbers is still an open question. The presence of buffer zones even three times as long as the porous domain was still not able to completely mitigate the presence of fluid jets which can have important applications in fluid and contaminant mixing and heat transport at the contact between the porous domain and the free fluid domain.

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Poster / 1040

Development of multiphase flow simulation method in DEM under a movable-grain condition

Author: Quanwei Dai[1]

Co-authors: Fiona CY Kwok [2]; Kang Duan [3]

[1] *PhD Candidate*

[2] *Assistant Professor*

[3] *Professor*

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Understanding how hydrodynamics of multiphase flow couple porous media deformation is essential to ensure successful engineering practices such as geological carbon sequestration. However, existing hydro-mechanical coupled models face significant challenges in reliably and efficiently capturing fluid-grain displacement patterns. In response, we present a novel two-way coupled hydro-mechanical discrete-element method model that manages fast fluid transport and considers the synchronising pore deformation. This model, which employs the implicit finite volume approach to solve pore pressure under a remarkable timestep, predicts fluid-fluid and fluid-grain interactions unconditionally stable. We design a pressure-volume iteration scheme to balance injection-induced pressure changes with pore structure rearrangements dynamically. Additionally, we incorporate adaptive flow front advancement criteria to enhance the capture of interface motion, particularly in complex flow scenarios where fluid migration surpasses the frontline pores or is impeded by capillary effects. The robustness and reliability of our model, validated against Darcy flow theory and experimental observations from Hele-Shaw tests, demonstrate its capability in accurately analysing multiphase fluid migration and dynamic fluid-grain interactions in porous media. We are confident in considering this model a powerful tool to illustrate the micro-mechanisms of multiphase flow in deformable porous media.

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MS10 / 1041

Pore- and Nano-scale Imaging of Pore Changes During CO2 Injection in Sandstone

Authors: Rukuan CHAI[1]; Sepideh Goodarzi[2]

Co-authors: Anindityo Patmonoaji [2]; Martin J Blunt [2]; Branko Bijeljic [2]; Anfal Al Zarafi [2]

[1] *Imperial College London*

[2] *Department of Earth Science and Engineering, Imperial College London*

Corresponding Authors: a.patmonoaji@imperial.ac.uk, m.blunt@imperial.ac.uk, sepideh.goodarzi19@imperial.ac.uk, b.bijeljic@imperial.ac.uk, a.al-zarafi23@imperial.ac.uk, r.chai@imperial.ac.uk

We employed X-ray Computed Tomography (CT) and Scanning Electron Microscopy-Energy Dispersive Spectroscopy (SEM-EDS), alongside a steady-state flow experiment involving calcite-contained sandstone and pre-equilibrated fluids, to study the changes occurring in the pores of sandstone during CO2 injection. In-situ pore-scale imaging showed a significant increase in average porosity, from 23% to 28%. This increase was due to the formation of new pores and the enlargement of existing ones, which occurred earlier in proximity to the injection inlet. Concurrently, pore shrinkage is also observed, typically after the pore enlargement, affecting regions within small pores. The combined effect increased heterogeneity. SEM-EDS provides nano-scale insights, identifying calcite dissolution as contributing to new pore formation, feldspar fragmentation and clay migration as associated with pore enlargement. Furthermore, the blockages induced by clay or fragmented feldspar migration resulted in pore shrinkage. Thus, it is not only the reactive mineral, calcite, that plays a critical role, but also feldspar and clay exert significant influence. Our study clarifies the changes occurring in the pores during CO2 injection into sandstone and highlights the influence of mineral composition on geological CO2 sequestration.

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1042

Computation of Permeability matrices from Human coronary artery

Authors: Jacques Huyghe[1]; Kunal Nath[None]

[1] *University of Limerick/Eindhoven University of Technology*

Corresponding Authors: jacques.huyghe@ul.ie, kunal.nath47@gmail.com

Permeability plays a crucial role in regulating blood flow and nutrient exchange within the coronary circulation. This study presents a MATLAB-based computational model to analyse permeability variations across the coronary vasculature. Utilizing cryomicrotome imaging data obtained from the University of Amsterdam, we reconstruct a 3D representation of the coronary network. A detailed permeability calculation, incorporating vessel position, diameter and length, is applied to each vessel segment. We demonstrate significant permeability heterogeneity across different vessel sizes. Furthermore, by classifying vessels based on key arteriovenous parameters, we uncover distinct permeability patterns within specific functional ranges. This work, conducted in MATLAB, advances our understanding of coronary blood flow dynamics and holds potential for improved modelling of cardiovascular health and disease.

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1 Schwarz JCV, van Lier MGJTB, van den Wijngaard JPHM, Siebes M and VanBavel E (2020) Topologic and Hemodynamic Characteristics of the Human Coronary Arterial Circulation. Front. Physiol. 10:1611 2 Jacques M. Huyghe, Cess W. Oomens, Dick H. van Campen, Robert M. Heethaar (1989) Low Reynolds Number Steady State Flow Through a Branching Network of Ridgid Vessels: I. A Mixture Theory BIORHEOLOGY, 26; 55-71, 1989

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Poster / 1043

Monitoring nano-scale fluid films in porous rock with AFM

Author: Maja Ruecker[1]

Co-authors: Gijs Wensink [1]; Mehrbod Keshavarzi [2]; GEORGE CLADUIU SAVULESCU ; Paul Luckham [3]

[1] *Eindhoven University of Technology*

[2] *PhD Student Imperial College*

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During fluid displacement in porous rock or soils, as they occur in aquifers or other fluid reservoirs such as CO2 or H2 storage sites or hydrocarbon reservoirs, water films form along the internal pore surface of porous rocks due to its wetting properties and capillarity. Near connate water saturation, these water films dominate the macroscopic flow behaviour as observed e.g. in relative permeability experiments.
We use Atomic Force Microscopy (AFM) to study the sub-pore scale configuration of microscale water films on the rough pore surface of Ketton and Estaillades rocks to illustrate the potential of AFM to qualitatively assess the nature of such fluid films at different static and dynamic conditions. Experiments were performed on model systems to test the methodology of AFM fluid film measurements 1. The static conditions include measurements after drainage, alteration of the surface with crude oil and water flooding. The dynamic conditions include spontaneous imbibition and drying cycles 2. The experiments were compared to various computational models and macroscopic responses monitored with micro-computed tomography data [2,3].
The results show that the nano-scale water films forming along the internal surface of porous rocks, facilitate corner flow as described by [4] rather than a thin continuous layer of water along the surface frequently assumed [5]. We notice that the water coverage along the pore walls surface shows a variation in continuity and depth depending on the preconditioning of the sample. The results showed that water films can prevail the wetting alteration process. However, only one out of three crudes provided evidence for such water films. The measurements after the water flood further revealed water entrapped by an oil layer as well as regions of different adhesion following a pattern

similar to the water distribution observed prior to the wetting alteration. The dynamic scans indicate swelling and shrinkage, which may relate to larger sale pore-scale displacement events in other regions.
The combination of different experimental studies illustrates the capacity of AFM to inform us about the behaviour of nano-scale fluid films during multiphase flow in porous media. Whereas quantitative estimates remain difficult due to the small scanning area, this methodology can provide insights into the mechanisms of fluid film formation, swelling and shrinkage during multiphase flow in porous rock.
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[5] T. C. G. Kibbey, The configuration of water on rough natural surfaces: Implications for understanding air-water interfacial area, film thickness, and imaging resolution. Water Resour Res 49, 4765–4774 (2013).

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Poster / 1044

Gas-water two-phase hydro-mechanical coupling simulation in deep shale considering nanomicroscale effects

Authors: Dongying Wang[1]; Hua Liu[1]; Xiaohu Hu[1]; Yanyan Wang[1]

[1] *Petroleum Exploration and Production Research Institute, SINOPEC, Beijing, China*

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The depth of deep shale gas reservoir is greater than 3500m, the initial liquid production of gas well is large and the flowback rate is high, accounting for the complex gas-water two-phase transport behavior. Besides, due to the characteristics of high pressure and stress in deep shale gas reservoir, the existing transport simulation method is no longer applicable. In this work, a hydro-mechanical coupling simulation method of gas-water two-phase transport in deep shale gas reservoir with respect to the pore, core, and field scale is proposed. First, the fluid storage state and transport behavior in different pore types during the gas–water two-phase transport process is investigated, with incorporations of 1) real gas transport controlled by Knudsen Number (Kn) and second-order slip boundary, 2) slip length for water phase transport, 3) a mobile water film with varying thickness due to rock-fluid interaction and 4) stress-dependence. Subsequently, the gas–water two-phase transport

behaviors are upscaled from the pore to the core by incorporating nanomicroscale effects through fractal model. Next, an adaptive hybrid model is used to simulate the hydro-mechanical coupling in multi-scale fractured deep shale gas reservoirs, in which hydraulic fractures are modeled explicitly by using the embedded discrete fracture model, and micro-fractures are modeled by using the continuum models. Moreover, gas-water two-phase transport behaviors in fracture system is obtained in laboratory, and matrix core-scale transport behaviors are incorporated in the macroscale model. Finally, the influences of nanomicroscale effects, stress filed, bottom hole pressure and fracturing parameters on the production of shale gas reservoirs are discussed comprehensively. This study provides a practical method to estimate deep shale gas production by rigorously considering gas–water nanomicroscale effects and geological characteristics to reduce uncertainties during productivity evaluation.

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Poster / 1045

Thermo-hydro-mechanical coupled zero-thickness interface finite elements: benchmarking and application

Authors: wen luo[None]; Joaquin Liaudat[1]; Josselin Ouf[2]; Anne-Catherine Dieudonné[3]; Florian Amann[4]; Philip J. Vardon[3]

[1] *Technical University of Darmstadt*

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Coupled thermo-hydro-mechanical (THM) processes play a key role in subsurface use, e.g. geothermal energy, CO2/H2 storage and geological repository. However, understanding these processes in porous media, in which natural fractures can be present and new fractures can be induced, is non-trivial task. The Cohesive Zone Model (CZM), a numerical technique in the framework of the Finite Element Method (FEM), is one of the possible choices in modelling fracture initiation and propagation due to its simple physical meaning and its mitigation of the need to calculate the stress singularity at the fracture tips that is commonly challenging in methods based on classical linear elastic fracture mechanics. In this work, we developed a THM coupled zero-thickness interface finite element employing CZM. It is developed to allow the simulation of longitudinal and transversal fluid/heat flow inside the fracture. The cubic law is used to simulate the fracture transmissivity as a function of its aperture, while an elasto-damage law is used to characterise the mechanical response of the discontinuity. The method is successfully verified against two analytical solutions: one of the coupled thermo-hydraulic response of a single fracture, and the KGD fracturing model that describes

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MS03 / 1046

Effect of mineral on mechanical behavior of granite after high-temperature treatment by particle flow simulation

Author: Yahua Wang[None]

Co-authors: Jiafang Xu ; Yongqiang Chen ; Bowen Wang ; Jian Wang ; Jie Chen

Corresponding Author: yahwang23@163.com

Understanding the effect of minerals on the mechanical behavior of granite under thermo-mechanical coupling is of great significance in deep engineering. In this paper, nine thermo-mechanical grain-based models of granite with different mineral contents were established based on particle flow simulation, revealing the influence mechanisms of temperature and mineral on the mechanical properties and micro-damage of granite. The results indicate that the macroscopic mechanical properties, micro-damage and failure mode of granite are synergistically affected by mineral, distribution and thermal properties. With increasing temperature, the thermally-induced cracks in the granite samples gradually gather from the edge towards the centre. The proportion of intergranular cracks in thermally-induced cracks is much greater than that of intragranular cracks. The stress concentration between mineral particles caused by the temperature increase is the main cause of thermally-induced cracks.

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Poster / 1047

Numerical Simulation of the Microbial Induced Calcite Precipitation (MICP) Process in Darcy-scale and Pore-scale

Author: Dianlei Feng[1]

Co-authors: yajie chu [1]; Lingxiang Wang [1]

[1] *Tongji University*

Corresponding Author: dianleifeng@163.com

Microbial Induced Calcite Precipitation (MICP) technique is a “green” bio-grouting method developed in recent years, which has been applied in many engineering fields. The MICP technique has attracted extensive attention due to its high reinforcement strength and environment-friendly properties. However, MICP reinforcement often faces the problem of non-uniformity precipitation, which happens in different spatial scales and is one of the bottleneck problems restricting the further development of this technology. In this study, the uniformity of calcium carbonate precipitation in the MICP process has been studied numerically in both the Darcy-scale and the pore-scale. The influence of grouting injection strategy, non-uniform distribution of soil material properties, and pore characteristics on the uniformity of MICP reinforcement have been preliminarily investigated.

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Poster / 1048

Multi-scale characterization for pore systems of hydrate-bearing reservoir ——Kerishna-Godavari Basin, India

Author: 文管[1]

[1] *Peking University*

Corresponding Author: 2001110630@pku.edu.cn

The microscopic pore system of hydrate-bearing sediments in the KG Basin was thoroughly described using X-ray computed tomography (XCT), low-field nuclear magnetic resonance (NMR), and N2 gas adsorption (N2GA) technique. Results indicate that the pore types are intricate, exhibiting a wide range of pore shape and limited connectivity. Foraminiferal shells contribute to the presence of certain pores, whereas micropores ranging from 4-20μm play a significant role in determining permeability. The absence of measuring closed pores with N2GA resulted in a notable disparity in the overall pore volume when compared to NMR findings.
NMR technique is used to monitor the phase transition process in pores as the temperature changes. The intensity value of the first peak signal of CPMG is measured, and the pure water signal is used as a reference to compute the amount of unfrozen water and the distribution of pore sizes. It is found that the water signal within the macropores is consistently rising, although it is considerably weaker compared to the micropores. The peak values in the mesopores, which belong to the medium range, are disordered. Analysis indicates that water migration takes place within the mesopores. The initial process of ice melting into water occurs within smaller holes.

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Poster / 1049

Adsorption Swelling and Anisotropic Characteristics of CO2 in Shale

Authors: Shuangshuang Lin[1]; Xin Chang[1]

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Abstract. Geologic sequestration of carbon dioxide (CO2) is one of the most significant technologies to combat climate change at present. Nevertheless, the CO2 injected into shale reservoirs can expand to affect the permeability and strength of the reservoirs, affecting the efficiency of injection and the safety of storage. In this work, the strain behavior of He (1300 psi) andCO2 (850 psi) on shale samples at constant hydrostatic pressure was investigated using a self-developed high temperature and high pressure gas adsorption and expansion apparatus measuring temperatures at 308 K. The results indicate that adsorption expansion of CO2 exists in shale samples. With increasing pressure, the swelling rate increases and then decreases, and the adsorption-induced swelling strain of shale shows a Langmuir-like relationship with pressure. The adsorptive deformation of shale is anisotropic, with deformation perpendicular to the direction of the laminae being greater than that parallel to the plane of the laminae. The asynchronous response of adsorptive swelling and mechanical compression produced by CO2 gas can lead to crack expansion in rocks and rock fracture.

The amount of swelling is dependent on the CO2 concentration, and the swelling of shale is mainly determined by the partial pressures of the component gases.

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MS15 / **1050**

Integrating deterministic geological model with multimodal machine learning to predict shale productivity

Authors: Gang Hui[1]; Muming Wang[2]; Fuyu Yao[1]; Hai Wang[2]; Zhiyang Pi[1]; Penghu Bao[1]

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Over the past ten years, diverse machine learning techniques have been extensively employed in forecasting output for non-traditional reservoirs. Nevertheless, these techniques primarily utilized discrete point data obtained from field databases, such as well drilling, completion, monitoring, experiments, and production data of horizontal wells. However, this data fails to capture the spatial heterogeneity of reservoir properties, which ultimately undermines the reliability of shale gas production. This study proposes a multimodal machine learning approach that utilizes a geological model restricted by well-logging and 3D seismic data. The deterministic geological model is constructed by utilizing the high vertical resolution of well logs and the planar resolution of reflection 3D seismic attributes. Subsequently, the detailed and precise data regarding geological properties such as porosity, permeability, gas saturation, TOC, brittleness, thickness, etc. in the vicinity of horizontal wells are acquired using the aforementioned geological model. These data are then combined with traditional tabular datasets to accurately represent the heterogeneity of the reservoir. Subsequently, a multimodal model is created that combines a convolutional neural network (CNN) module and an artificial neural network (ANN) module. The CNN module is designed to handle high-level information from the visual dataset, while the ANN module is used to evaluate the typical tabular datasets. A fusion module integrated and processed input from both modalities. The results demonstrate that the multimodal approach attained a coefficient of determination (R2) of 0.845 for the 12-month shale gas production prediction, which is greater than the R2 value of 0.721 obtained using simply the ANN model. In addition, this approach based on the multimodal of analysis can elucidate the varying levels of shale gas production between two horizontal wells that have similar average reservoir attributes. This is achieved by taking into account the lateral heterogeneity of the producing formations that the two horizontal wells have penetrated. Hence, the exceptional predictive accuracy of the multimodal machine learning technique offers valuable insights into forecasting shale gas production. This approach may be utilized to guide the selection of optimal locations for new horizontal wells and facilitate the efficient exploitation of shale gas reservoirs.

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1051

Study of seepage damage by wax precipitation from highly waxy crude oil in low permeability reservoirs

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In highly waxy oilfields, deteriorating conditions like changes in crude oil composition, temperature, flow rate, and pressure cause wax crystals to precipitate from the crude oil. This poses significant challenges for oilfield production and transportation.This paper examines the wax damage of highly waxy crude oil in low-permeability non-homogeneous reservoirs by analyzing the flow properties

and recovery rate changes using a high temperature rheometer, oil-water phase permeability instrument, and crude oil seepage cold damage device. Additionally, we study the number and morphology of wax crystals precipitated from the crude oil at different temperatures using a high magnification microscope. Furthermore, we analyze the distribution of microscopic stagnation of the waxed crude oil and validate the seepage results by utilizing a scanning electron microscope. The Scanning electron microscope (SEM) is employed to investigate the micro retention distribution of waxy crude oil and to confirm the seepage results of highly waxy crude oil.When the temperature drops below the wax precipitation point, the formation of large and stable three-dimensional wax crystals from individual particles occurs, leading to an increase in the viscosity of the crude oil. This transformation results in the crude oil becoming a non-Newtonian fluid, impeding its flow. In the reservoir rock, the wax crystals that precipitate may adhere to the surface of rock pores, causing a reduction in the diameter of the rock pores. This action restricts the flow of crude oil. Additionally, the wax crystals can mix with macromolecules in the tiny pores and channels of the rock, creating blockages that lead to accumulation and damage from wax precipitation.To enhance the development of high wax-containing crude oil, a priority is to mitigate the adverse impacts of wax deposition by improving the reservoir fluid seepage capacity. Specifically, when the temperature surpasses the wax precipitation point, the heterogeneous droplet structure of the crude oil can help reduce the resistance to oil seepage. During the production process, with an increase in temperature, the crude oil viscosity decreases leading to a shift of the oil-water relative permeability curve upwards and to the right. Consequently, the area of the two-phase co-permeability region expands, resulting in enhanced crude oil recovery rates. The findings of this study contribute to a better understanding of wax precipitation deposition and suppression during lifting operations, offering valuable theoretical insights for exploiting high wax content crude oil through thermal oil recovery techniques.

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MS13 / 1052

Molecular simulations of Cavitation Bubbles dynamics

Author: Yuequn Fu[1]

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The observation of a cavitation bubble forming as a nano-scale spherical surface detached from a flat substrate unveiled complexities in capturing the cavitation pattern, hindered by existing methodological constraints. To decode the molecular dynamics and detailed morphology underlying this phenomenon, the study applies molecular dynamics (MD) simulations. This investigation mapped the onset and early development stages of cavitation at the nanoscale, organizing the morphology into four distinct phases and highlighting a pivotal moment where the rates of nucleation and growth find equilibrium. The research further explores the effects of variable pulling speeds and ambient pressures on the dynamics of cavitation through simulations. It was observed that higher pulling

speeds amplify the cavitation volume but reduce the bubble's lifetime. On the other hand, ambient pressure variations significantly influence both the maximum volume and the collapse rate of the cavitation. The findings are systematically encapsulated in a phase diagram that displays the effects of varying pulling speeds and ambient pressures. Significantly, the study corroborates a Family-Vicsek scaling law, predicting the maximum volume and lifetime.

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MS15 / **1053**

Super-resolution imaging of multiphase fluid distributions in porous media using deep learning

Author: Zhuangzhuang Ma[None]

Co-authors: Branko Bijeljic [1]; Gege Wen [2]; Kunning Tang [3]; Martin Blunt [4]; Yang Gao [5]

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X-ray imaging has become an indispensable tool in the study of porous media, significantly enhancing our understanding of multiphase flow within these pore structures. High-resolution X-ray images enable researchers to accurately measure or calculate critical rock properties such as porosity, interfacial surface area, curvature, and contact angle distributions. These images are also pivotal in determining capillary pressure from local interfacial curvatures. Achieving high-resolution images with a large field of view (FOV) is crucial for obtaining accurate and representative geometrical and physical properties, yet balancing FOV with resolution remains a formidable challenge. Recently, super-resolution imaging techniques using deep learning have demonstrated considerable potential in addressing this issue. We have successfully implemented an Enhanced Deep Super-Resolution (EDSR)-based method on multiphase flow images, which produced high-resolution results while expanding the FOV. A rigorous comparison with ground truth confirms that our super-resolution outcomes are consistent with the ground truth. This breakthrough is particularly significant as it provides more detailed and expansive insights into fluid behaviour in porous media, thereby paving the way for future advancements in geological research and practical applications.

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Poster / 1054

Research on the occurrence states of microscopic remaining oil in ultra-low permeability reservoirs

Author: Huaimin Dong[1]

Co-authors: Peng Chi [2]; Bo Dai [3]; Jian Zhuang [3]; Likai Cui [4]

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The Chang 6 reservoir represented by Wangyao Area in Ansai Oilfield is the earliest developed reservoir in Changqing Oilfield. After nearly 40 years of exploration and development, the comprehensive water cut has reached 72.8%, and the degree of geological reserves recovery is only about 17.8%. The reservoir has entered the middle and late stage of development, and the reserve-production ratio has decreased year by year, and the problems of production decline and low recovery degree have become more and more serious. The effect of conventional water flood adjustment and cyclic water flooding are not obvious. So it is necessary to use polymer injection, phlogisticated air injection and carbon dioxide injection to enhanced oil recovery. However, due to the great differences in the micro-pore structure of the reservoir, the location and shape of the micro-remaining oil are different, and the corresponding tapping methods for different types of micro-remaining oil are also significantly different. Therefore, it is necessary to carry out systematic water drive experimental research on the ultra-low permeability reservoir whose micro-remaining oil occurrence characteristics and production mechanism are not completely clear at present. In this study, the ultra-low permeability lithology reservoir of Chang 6 formation in Ansai Oilfield was taken as the research target area. By using the dynamic displacement scanning technology to obtain two-dimensional image information of micro-plunger core in different water flooding stages, and reconstruct the occurrence states of micro-remaining oil in three-dimensional pore space, and the types of micro-remaining oil were divided and quantitatively calculated according to its formation mechanism and three-dimensional structural parameters. Furthermore, the types and dynamic changes of micro-remaining oil in different water drive stages are analyzed, and the potential of micro-remaining oil in different development stages and corresponding utilization methods are defined, in order to provide theoretical guidance for the smooth implementation of water drive and tertiary oil recovery in ultra-low permeability reservoir.

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Poster / 1055

3D multi-scale reconstructed structure and transfer properties of porous material based by multiple approaches

Author: Xiaoyan MA[1]

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The micro and nano structures of porous material have strong influence on their transfer properties such as porosity, permeability, tortuosity and adsorption isotherm curves. In the construction and building material field, these properties are strongly related to hydro and thermal comfort, due to the fact that heat and mass transfer mechanisms are determined by the micro porous structure. In the present work, we aim to predict heat and mass transfer on such micro-nano structured materials, with a statistical quantification method that is extracted from morphology aspect. A large range of the pore size (from 20nm to 1mm) is covered and investigated by the multiple approaches, including FIB-SEM, X-Ray Tomography, and MIP (Mercury Intrusion Porosimetry). The 3D view of pore structures are obtained in concrete, as well as their size distribution, and pore zones. A reconstruct of 3D view of pore networks is extracted, with the spatial resolution of 20 nm/pixel. A global view of multiple testing methods and the corresponding size ranges are drawn to summarize the multi-scale approaches, for a potential further understanding of relationship between porous structure and thermal-hydro properties.

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Poster / 1056

Improving chemo-mechanical properties of wellbore cement for deep wellbore conditions in the presence of CO2

Author: Chigbo Waliezi[1]

Co-authors: Dirk Engelberg [2]; Majid Sedighi [2]; Mojgan Hadi Mosleh [3]

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Abstract
In recent times given the wealth of advancement in scientific research, scientific evidence has shown that CO2 accounts for over 75% of greenhouse gas emission rise between 1990 and 2021 and is projected to further increase due to increasing energy demands in developing countries. Amongst several mitigation tools, The CCS stands out as the most efficient mitigation tool and is projected to reduce CO2 emission by over 20% in 2020 and about 55% cumulatively by 2100.
However, CCS application in its final stages encounters an imminent challenge of unwanted CO2 leakage and fluid migration through the agencies of geological and engineering pathways. While geological pathways account for leakages credited to altercations of geological reservoir play elements similar to conventional petroleum wells, engineering pathways consist of leakages credited to wellbore integrity-related issues, encompassing all wellbore integrity systems such as the casing program, well cementing design program, and material selection which is the focus of this study. CO2 leakage accounted for by wellbore integrity-related issues occur due to the carbonic acid vulnerability of Portland cement seal, credited to the chemical interaction of CO2, formation water, with in-place cement sheath. As diffusion drives chemical interaction, it is further propagated by default cement sheath transfer properties with carbonation front expanding into cement core completing a series of calcium hydroxide precipitation, bicarbonation, and eventual cement matrix leaching, leaving a depleted cement sheath characteristic of low mechanical strength and degraded gas and fluid migration barrier systems.
Several advances have been made in literature in the last decade, especially in conventional petroleum wells in CO2-rich environments, such as the alteration of cement-to-water ratio, use of non-portland cement, application of special cements and application of pozzolanic materials all of which unfortunately range from high-cost complication to durability deficiencies and thus, allows for continuing research.
This research focuses on developing a chemo-mechanical efficient cement composite suitable for geologic sequestration through a CO2 mechanism of degradation inclined method development, and thus consists of concept building, determination of key performance areas for an efficient cement sheath, identification and characterization of high-performance single material additives through

secondary and experiment-based data analysis, and development of hybrid additives based on high performance, mechanism and compatibility exploring petrophysical, physical, mechanical, and chemical analysis sets geared towards efficient and effective performance and characterization. Results of the chemical composition show significant chemical potential for strength improvement and acid resistance by diffusion inhibition, while Results of the chemical composition show significant chemical potential for strength improvement and acid resistance by diffusion inhibition. The outcome of the study will proffer a tripartite enhancement intervention across chemical, petrophysical, and mechanical properties of wellbore cement sheath.

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1057

Research on Remaining Oil Distribution Based on Fine Anatomy of Reservoirs

Author: Dong Ma[None]

Co-authors: Chao Li [1]; Hanqing Zhao [1]; Hua Dan [1]; Huijiang Chang [1]

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1708 sand body in the lower member of the Neogene Minghuazhen Formation is a structural-lithological reservoir developed by horizontal wells, which is typical of meandering fluvial deposits. Contradiction of dynamic production performances occurred after it went into production, wells in its northwestern part flowed with high yield with no water, whereas wells in the southern part were pumped with low yield and water cut increased quickly up to 80%. Causes were analyzed based on seismic, well logging, drilling and dynamic data. Oil flowed to surface in Well A9 and A12H of the northeastern part due to edge water drive, A12H was also affected by gas cap. A15H and A16H were located in the southern part near edge water, which led to rapid rise of water cut due to secondary bottom water caused by quick breakthrough of edge water. Therefore, areal and vertical heterogeneity is the main influencing factor bringing about the contradiction of dynamic production performances between southern and northern part. Based on above understandings, remaining oil distribution was analyzed.

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Poster / 1058

Coupling reaction transport model and multiphase hydrate simulator for studying anaerobic oxidation of methane

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The anaerobic oxidation of methane (AOM) occurring in the surface sediments acts as an important barrier to methane emissions, caused by the reaction between sulphate ions and dissolved methane molecules. However, the current hydrate simulators rarely consider the transport of sulphate and the subsequent AOM reaction. In this study, to investigate AOM effects in hydrate systems, a new simulator named Tough+Hydrate+AOM (THA) is developed by combining the reaction transport model with the widely-used Tough+Hydrate simulator. The THA simulator is validated using the single-phase cases of the Dvurechenskii mud volcano in Black Sea, since the results obtained are in good agreement with previous ones. The THA simulator considering AOM is expected to be an important tool for assessing methane emissions caused by hydrate destabilization.

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Poster / 1059

A Theoretical Model for Thermal Conductivity of Fibrous Porous Media

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Thermal conductivity is a fundamental physical property in porous media, and is critical to various industrial applications. Most existing theoretical models appeal to estimate thermal conductivity with isotropic assumption and the applicable conditions are relatively rigorous. This paper introduces a theoretical model that evaluates the thermal conductivity of fibrous porous media. The model is based on Fourier's Law and involves a complex thermal resistance circuit analysis, considering the direction of heat flux originating from the X, Y, and Z axes within the Cartesian coordinate system. The proposed model was found to be reasonable upon comparison with existing models. By comparing the effective thermal conductivity calculated by the model with results obtained from Computational Fluid Dynamics (CFD) and discrete numerical solution methods, the high accuracy of the model has been validated. The extension of the proposed model based on fractal theory was also discussed. It is anticipated that the proposed model will offer an alternative approach to computing the thermal conductivity and figuring out the mechanism of heat transfer behavior in fibrous porous media.

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Poster / 1060

Effect of elevated-temperature on mechanics and microstructure of basalt fibre-modified cementitious composites

Author: HAO HAN[1]

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Cementitious materials, known for their brittle nature, are often vulnerable to thermal degradation in deep underground and hydrothermal environments. Basalt fiber (BF), an inorganic silicate additive used in cement, has garnered significant attention due to its outstanding mechanical and thermal resistance properties. However, key experimental data are scarce on the role of BF in cement exposure at elevated-temperature conditions, and a lack of understanding of the key mechanisms of reinforcement processes. In this study, we investigate the mechanical behavior of cementitious composites with varying BF content under both ambient and elevated temperature conditions (up to 200℃) to determine the optimal dosage. Microstructural analysis and phase composition assessments are conducted to reveal the mechanisms of reinforcement, encompassing the state of the cement matrix, BF

itself, BF-matrix interaction, and phase evolution. The results indicated that the addition of 0.05-0.1 wt.% BF to cement can significantly enhance its mechanical strength and crack resistance, with flexural strength improving by up to 60% after exposure to 200℃ for 6 days. This enhancement is primarily attributed to multiple energy-consumption processes, including the bridging effect, breaking effect, pulling-out effect, crack deflection effect and adhesive effect. Notably, the adhesion between BF and the cement matrix improves after exposure to 200℃, leading to the formation of "network-like and granular hydration products" on the surface of BF. While needle-like hydration products are commonly observed under ambient conditions, contributing to a slight increase in the surface friction of BF, the accelerated growth of hydration products at higher temperature conditions emerges as the predominant factor enhancing mechanical strength and improving ductility of cement composites at elevated temperatures. The insights from this study provide promising prospects for the application of BF-modified cement composites in elevated-temperature environments, including deep geothermal wells, CO2 storage wells, and various other deep geo-energy applications.

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Poster / 1061

Non-invasive imaging of solute redistribution below evaporating surfaces using 23Na-MRI

Author: Mohammad Ali Chaudhry[None]

Co-authors: Andreas Pohlmeier [1]; Johan Alexander Huisman [2]; Rainer Helmig [3]; Stefanie Kiemle

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Evaporation from porous media is a key phenomenon in the terrestrial environment and is linked to accumulation of solutes at or near the evaporative surface. It eventually leads to salinization, soil degradation and weathering of building materials, topics with high economic impacts. Although the detrimental effects manifest on different scales from pores to the field, the key to understanding is found on the pore scale since pore system connectivity and structure control the solution behavior near the evaporation surface. A thorough understanding requires the development of physical models describing the most relevant processes and their validation by experiments. Vice versa, new experimental observations promote the further development of the physical models.
In this context, the current study aims at the understanding of solute accumulation near evaporating

surfaces for model porous media at the cm-scale. Analytical and numerical modelling predict the development of local instabilities due to density differences during evaporation in case of saturated porous media with high permeability, which eventually causes density-driven backflow through fingering [Bringedal et al. TPM 2022]. To experimentally investigate this process, we performed experiments on sand packings with a diameter of 3.1 cm and a height of 4 cm prepared with two types of porous media: F36 (medium sand) and W3 (fine sand/silt) with porosities of 0.37 and 0.39, respectively. The intrinsic permeability of the two packings differed by two orders of magnitude, i.e. 2.9×10-11 m2 for F36 and 5.6×10-13 m2 for W3. Using magnetic resonance imaging (23Na-MRI), we monitored the development of solute accumulation and subsequent backflow with high spatial (1 mm) and temporal (1 hr) resolution during evaporation with a continuous supply of water at the bottom of the samples (wicking conditions).
Significant differences between the 23Na enrichment patterns were observed for the two types of sand. F36 sand produced an initial enrichment at the surface within the first hour, but soon after a downwards moving plume developed, hence redistributing NaCl back into the column. This was attributed to density driven backflow made possible by the high permeability. The backflow caused a good mixing of the solute during the observation period of 120 h. 1D concentration profiles with depth obtained from the 3D imaging showed that the average concentration reached only 2.5 mol/L, well below the solubility limit of 6.13 mol/L. In contrast, for fine W3 sand with lower permeability, enrichment only took place in a shallow near-surface zone of a few mm with a maximum concentration of 5.1 mol/L after 73 hours of evaporation. No fingering occurred although the mean evaporation rate was similar to that of the F36 sand. These results highlight the major role that porous media properties play in solute redistribution near evaporating surfaces, which was predicted by theory and now confirmed experimentally. The findings encourage further investigations involving different porous media with systematic variation of hydrological properties and the coupling of experimental results to numerical modelling.

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MS13 / 1062

Smart Water Flooding: Experimental study and Molecular Simulation

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In the background of the strong oil wettability and low production by water flooding in carbonate reservoirs, low salinity water containing sulfate ions and nanoparticles can significantly change the surface wettability of carbonate rocks and thus increase the sweeping area, however, the absorption and desorption mechanisms of the oil film in the carbonate rock surface remain unclear. In this

work, These problems is addressed in the framework of molecular dynamics simulation (Material Studio software) and experiments. The results were showed that sodium sulfate solution could accelerate the rate from oil-wet to water-wet and the interaction of oil molecules, water molecules, and SO42- ions at molecular scale was explained. The results of the simulations show that many water molecules travel down the water channel under the influence of several powerful forces, including the electrostatic force, the van der Waals force and hydrogen bond, crowding out the oil molecules on the calcite's surface and causing the oil film to separate.

At the same time, a hybridization technique of combining low salinity water and nanofluids was performed by using experiments such as contact angle measurement, core displacement, and NMR (Nuclear Magnetic Resonance), and the effects of different salinity water and the nanofluids concentrations on wettability alteration and enhanced oil recovery were revealed. The parameters of wettability changes and contact angle were measured at different nanofluid solutions with high/low salinity water. The experimental results revealed that the test with KCl-1+NF outperformed other compositions. As for the new method of hybridization technique, the insights presented in this study provide a good reference for further research in this area. In a word, these investigations can guide the practical application of low salinity water flooding in carbonate reservoirs.

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Poster / 1063

Pore-scale insights into CO2-water two-phase flow and implications for benefits of geological carbon storage

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The overall benefits of geological carbon storage (GCS) depend primarily on CO2 storability and injectability, expressed as saturation and relative permeability, respectively. The effects of GCS schemes on these two properties, the macroscopic response indicators of a two-phase seepage system, are closely related to pore-scale two-phase behaviors. However, the comprehensive effects of capillary number (Ca) and wettability (θ) on saturation and relative permeability are poorly understood. Here we proposed a digital rock physics (DRP) technique workflow for the phase field method and systematically investigated that how these effects control two-phase seepage at pore scale through the high-resolution visualization results obtained. We created a Ca-θ phase diagram identifying by four pore-scale displacement mechanisms, including finger-like invasion, burst, cooperative filling and coexistence of concave and convex interfaces, to illustrate the comprehensive effects of Ca and θ. We found that the relative permeability of the defending phase (water in this work) is determined by the net effect of the direct driving and viscous coupling effects. We organized comprehensive Ca-θ diagrams and revealed that a higher Ca and higher θ condition favors CO2 injectability, and a lower Ca and weak water-wetting condition favors CO2 storability. Our results demonstrate that GCS schemes, mainly about capillary number and wettability, can significantly influence CO2 storage performance via the two-phase flow at pore scale, which should be considered

carefully. This work provides valuable insights into the selection of an optimal GCS scheme and contributes to an in-depth understanding of multiphase seepage at pore scale.

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Breaking the classical approach: achieving homologous topology modulation of Hydrogen-Bonded Organic Frameworks

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Classical synthesis of hydrogen-bonded organic frameworks (HOFs) involve several steps, making challenging the systematic construction of isoreticular HOFs, due to the flexibility and easily disruption of the connection linkages be-tween OLs.1 Herein, we develop an "integrated synthesis-assembly"(ISA) methodology for constructing a series of homologous topological DAT-C6-HOFs (-1, -2 and -3) by minimizing the possibilities of being disrupted during the synthesis and assembly of HOFs. The pore sizes and microenvironments of the yielding DAT-C6-HOFs can be tuned by varying the structural modulation of π-bridge on C3-symmetric cyano-precursors (C3-CPs). Moreover, the obtained DAT-C6-HOF-1 exhibited highly selective sensing towards perfluorooctanoic acid (PFOA) among homologous molecules, based on the matched of pore size and the synergistic regulation of intra- and inter- molecular charge transfer excited states. The definition of the ISA method not only provides new ideas for the de-velopment of synthetic methods for DAT-HOFs and other kinds of HOFs, but also opens up new avenue for the derivation of the templates for the oriented as-sembly of HOFs as well as the structural modulation of HOFs.

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Poster / 1067

Lanthanide metal-organic frameworks as ratiometric fluorescent probes for real-time monitoring of PFOA photocatalytic degradation process

Author: Mingzhe Song[1]

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The assessment of perfluorooctanoic acid (PFOA) photocatalytic degradation usually involves tedious pre-treatment and sophisticated instrumentation, making it impractical to evaluate the degradation process in real-time. Here-in, we synthesized a series of lanthanide metal-organic frameworks (Ln-MOFs) with outstanding fluorescent sensing properties and applied them as luminescent probes in the photocatalytic degradation reaction of PFOA for real-time evaluation. As the catalytic reaction proceeds, the fluorescence color changes significantly from green to orange-red due to the different in-teraction mechanisms between the electron-deficient PFOA and smaller ra-dius F- with the ratiometric fluorescent probe MOF-76 (Tb: Eu=29:1). 1 The limit of detection (LOD) was calculated to be 0.0127 mM for PFOA and 0.00746 mM for F-. In addition, the conversion rate of the catalytic reaction can be read directly based on the chromaticity value by establishing a three-dimensional relationship graph of G/R value-conversion rate-time (G/R in-dicates the ratio between green and red luminance values in the image.), al-lowing for real-time and rapid tracking of the PFOA degradation. The recov-eries of PFOA and F- in the actual water samples were 99.3-102.7% (RSD=2.2-4.4%) and 100.7-105.3% (RSD=3.9-6.8%), respectively. Both the-oretical calculations and experiments reveal that the detection mechanism was attributed to the photoinduced electron transfer and energy transfer be-tween the analytes and the probe. This method simplifies the sample analy-sis process and avoids the use of bulky instruments, and thus has great po-tential on the design and development of quantitative time-resolved visuali-zation methods to assess catalytic performance and reveal mechanisms.

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Poster / **1068**

Study on the parameter in Unconventional Energy Reservoir Based on CT Scanning

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Unconventional energy sources refer to forms of energy obtained through methods distinct from traditional approaches (Demirbas, 2016). These include not only renewable resources such as solar and wind energy but also less conventional sources like gas hydrate and tar sands. The significance of unconventional energy lies in its potential to diversify energy supplies and reduce dependence on conventional fossil fuels, marking a critical shift towards more sustainable energy practices.

The study of the micro-properties of unconventional energy reservoirs, as emphasized by Bera and Shah (2021), is essential for a comprehensive understanding of their intricate pore structures and the characteristics of fluid flow within these formations. This deep understanding is fundamental to refining extraction techniques, boosting energy recovery, and diminishing the environmental footprint of such activities. It underscores the importance of such studies in the realm of sustainable energy development.

In particular, the investigation of porosity in these reservoirs is of paramount importance. As Zou (2017) highlights, understanding the porosity is key to grasping the storage and permeability capacities of these reservoirs, which in turn has a direct and profound impact on the efficiency of resource extraction. High-precision porosity analysis is instrumental in evaluating the quality of these reservoirs and in formulating the most effective and sustainable extraction strategies.

The evolution of science and technology, particularly with the advent of electronic computing and the introduction of industrial CT (Computed Tomography) instruments, has offered robust technical support for the microscopic examination of various phenomena within the porous media of unconventional energy reservoirs. This technological progression has been pivotal in advancing our understanding and capabilities in this field.

Initially employed in the realm of medical diagnostics, where its revolutionary impact was first recognized by Seeram (2018) and Withers et al. (2021), CT scanning technology, specifically Medical CT (MCT), has since transcended its original application. At the close of the 20th century, the introduction of industrial CT instruments marked a new era in geological research. Pioneering studies by Roth et al. (1998) and Vogel and Roth (1999) employed specialized CT scanners to produce a series of detailed color images of soil bodies, representing a significant breakthrough in the field.

However, the early stages of CT application in geological research were not without limitations. The initial CT instruments suffered from low resolution when scanning samples, posing challenges for detailed quantitative analysis. This limitation underscored the need for continuous technological enhancements to improve the resolution and accuracy of CT imaging, thus enabling more precise and detailed investigations of porous media. The evolution of CT technology has since seen substantial improvements, leading to its current status as a powerful tool for micro-level analysis and characterization, particularly in the complex and varied contexts of unconventional energy reservoirs.

This paper aims to delve into the refined methodologies and applications of CT scanning in the microscopic characterization of the parameter within unconventional energy reservoirs, highlighting its pivotal role in enhancing our exploration of these critical energy sources.

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