

InterPore2025



Report of Abstracts

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6

Study on microscopic mechanism of supercritical CO₂ flooding of shale oil in complex pores

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In view of the microscopic mechanism of CO₂ flooding shale oil in the process of oil development, the microscopic oil displacement model of CO₂ molecules in parallel connected pores and non-connected pores is established. The molecular dynamics simulation method is used to study the microscopic behavior of CO₂ flooding shale oil. The results show that the alkane in the connected pores will form a layer of high density adsorption layer in the middle of the pores during adsorption, and the distribution of free alkane in the connected pores will be more than that in the non-connected pores. The interaction energy between the shale oil and the wall in the organic pores is large, and the CO₂ in the organic pores is easy to form a fingering phenomenon during the oil displacement process. From the perspective of displacement efficiency, the displacement efficiency of connected pores is higher than that of non-connected pores. The displacement efficiency of organic connected pores is 5.91 % higher than that of non-connected organic pores. The displacement efficiency of inorganic connected pores is 1.96 % higher than that of inorganic non-connected pores. It can be seen that the influence of connectivity on organic pores is greater than that of connectivity on inorganic pores.

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Motion by beating of porous biofilms with heterogeneous rheology: Simulation and clinical assessment of therapy for cystic fibrosis

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Keywords and scope: mass transport in living systems, coupling of non-linear models, heterogeneous rheology, therapy monitoring, biological porous media, Stokes flow in moving geometries.

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

The system studied is a mucus made of Newtonian PeriCiliary Liquid (PCL) and highly concentrated mucins produced by the goblet cells, flowing through and above the epithelium ciliated cells (a porous medium described at its pore-scale, ie resolving the cilia individually), as shown on the joint figure. The cilia vibration generates a mixture between the mucins and the PCL, leading by reaction to a polymerized mucus with a heterogeneous rheology (space a time variable). Among the rheological features such as visco-elasticity, visco-plasticity, yield stress and shear-thinning, we focus on this last one which has been shown to be the dominant feature leading to non-functional mucus [3]. This leads to two-kinds of non-linearity whose effects compete or cooperate and provide functional or non-functional mucus propulsion.

The first non-linearity is the non-Newtonian pseudo-stationary Stokes equation driving the mucus motion, written $-div(2\mu(c, D) D(u)) = f - \nabla p$, where f is the driving force induced by the epithelial cell, μ is mucus viscosity, $D = (\nabla u + \nabla u^T)/2$ is the shear-rate of the velocity u , p is the pressure, and the incompressibility is satisfied by $div(u) = 0$.

Here $c(x, t)$ denotes the mucin concentration, and this Stokes equation is non-linear by means of the mucus shear-thinning rheology modeled by the Carreau law

$$\mu(c, D) = \mu_\infty + (\mu_0(c) - \mu_\infty) (1 + 2\beta(c)^2 |D|^2)^{\frac{q(c)-2}{2}}$$

The second non-linearity concerns the mucin concentration which satisfies a transport-diffusion model $\partial_t c + div(uc) - div(\sigma \nabla(c)) = 0$, since u can be written as a function of c . Beside, it can also been noticed that the diffusion becomes $-div(\sigma \varepsilon^{1+\tau} \nabla(\varepsilon^{-1} c))$ when upscaling the epithelium described as a porous medium (of porosity $\varepsilon(x, t)$ and tortuosity index τ).

We will show that numerical simulations using dedicated semi-Lagrangian methods [1,2] give good agreement with clinical picture of cystic fibrosis patients [4], whose sputum provides the rheological parameters. New clinical data also exhibit that simulations and sputum rheology allows to track pathology evolution for the patients under the recent triple-therapies.

This project MucoReaDy is funded by French National Agency of Research under the grant number ANR-20-CE45-0022.

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8

Controlled Haines jumps in a dual-channel multiphase system: inferring fluid properties from the dynamics of interface motion

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When one fluid is injected into a confined geometry such as porous media filled with another immiscible fluid, even at an extremely low injection speed, rapid filling of several pore spaces accompanied by retraction of multiple fluid-fluid interfaces can be observed. Such processes with fast liquid redistribution within the solid structure, called Haines jumps, are ubiquitous in many multiphase flow systems, which can impact fluid trapping, energy dissipation, and hysteretic saturation in various engineering applications. Inspired by this mechanism, here we propose a dual-channel structure to realise controlled Haines jumps during fluid displacement processes. Via theoretical analysis and numerical simulations, we show that the dynamics of fluid interfaces during Haines jumps can be quantitatively correlated with the driving capillary pressure and dissipating viscous stress, which enables simultaneous determination of the fluid viscosity and interfacial tension in the dual-channel multiphase system.

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The Impact of Anisotropic Reaction Rates on Dissolution Dynamics

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Mineral dissolution processes are prevalent in nature, yet the effects of anisotropic reaction rates, stemming from factors such as mineralogy and thermal gradients, still remain poorly understood. In this work, we leverage a level-set immersed boundary method to study reactive transport for a grain with heterogeneous reaction rates. Specifically, we analyze the major axis orientation, mass center displacement and eccentricity of the grain geometry during dissolution in the parameter space of Peclet number, Damköhler number and anisotropy factor. Our findings include a phase diagram that illustrates the transition between anisotropic and non-anisotropic effects. The results advance our understanding of the interplay between flow dynamics, reaction rates and anisotropy, thereby offering new insights into reactive transport.

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Fluid transfers through dynamic NMR relaxometry

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Nuclear Magnetic Resonance (NMR) relaxometry and Magnetic resonance Imagery (MRI) are well-established powerful tools for probing behavior of states of liquid in porous media. For years, the Navier laboratory has developed an innovative methodology to follow water transfer in porous media by this non-invasive and time resolved approach: dynamic NMR relaxometry (fig. (a), [1]), based on the fast exchange concept (fig. (b)) which distinguishes bulk and surface water at the pore scale. A full description of water transfer, such as drying of model nanoporous media like saturated Vycor [2] or biobased material as green wood [3] is facilitated by combining analyses of the evolution of the probability density function of the NMR relaxation time with profile of water content (1D MRI). More recently, this approach has been generalized to investigate liquid transfer in smoother material, such as clay paste or colloidal gel [4]. Once again, the fast exchange model provides a framework for translating NMR and MRI observable into key parameters evolution of porous and complex media, such as saturation, drying rate, volume fraction of paste or gel, effective pore size, specific “wet” surface or thickness of water film. This methodology enables the study of various drying regimes (shrinkage, desaturation, film formation...) independently, despite the complexities of medium deformations that may occur during liquid transfer.

Country:

France

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Student Awards:**Water & Porous Media Focused Abstracts:**

This abstract is related to Water

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Poster / 13

Complete Grain Segregation Under Submerged Conditions in a Rotating Drum

Author: Yu Chen¹

Co-authors: Deheng Wei¹; Yixiang Gan¹

¹ *The University of Sydney*

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Density-driven segregations in rotating drums, well-studied under dry conditions, reveal diverse symmetrical patterns due to variations in heavy and light grain densities (ρ_h , ρ_l) and rotating speeds (ω). Experimentally, we observe a complete segregation state in submerged systems, absent under dry conditions for the same ρ_h , ρ_l and ω . Simulations validated by experiments, using coupled computational fluid dynamics and discrete element methods, show that the mixing index can be accurately predicted across a wide range of effective density ratios, $D = (\rho_h - \rho_f) / (\rho_l - \rho_f)$ is the fluid density. As D increases, systems transition from well-mixed to fully segregated states, accompanied by an increasing number of vortices and more pronounced asymmetry. At higher Reynolds numbers (Re), the vortex area for heavy grains shrinks at lower D , while for light grains, it saturates; at higher D , an additional vortex appears in the light particle zone, expanding continuously. These findings provide new insights into segregation transitions in submerged granular systems and have implications for science and engineering applications.

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MS06-B / 15

Stochastic modeling of bacterial transport and retention in porous media

Author: Juan J. Hidalgo¹

Co-authors: Benjamin Piña¹; Claudia Sanz¹; Cristina Valhondo¹; Marta Casado¹

¹ IDAEA-CSIC

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Bacteria and microorganisms retention during water filtration allows to improve water quality and quantity. For that reason, the mechanisms affecting the propagation and fate of microbial populations need to be study to assess the risks for human health of water renovation technologies as managed artificial recharge.

In this work we study bacteria transport in porous media by means of column experiments. Two columns were built. One containing only sand and another with a mixture of sand, compost and wood chips. A punctual injection of tracers (rhodamine and amino-G acid) and bacteria consortium collected from the effluent of a wastewater treatment plant was made. Columns' outflow was sampled and analyzed to obtain breakthrough curves of the tracers and the different amplicon sequence variants (ASVs) of bacteria to determine the influence of columns' composition on the retention of bacteria. Bacteria and tracers displayed a strong anomalous behavior with late arrival peaks and long tails.

A continuous time random walk (CTRW) transport model was used to interpret the experimental results. The model characterizes transport in terms of mobile-immobile domains. Bacteria are transported with the mean flow and experience transitions from and to low mobility zones with a certain frequency. Transport is described in terms of four parameters, namely, the mean flow velocity, the dispersion coefficient, the trapping rate, and the mean residence time in the immobile zones. The model was able to reproduce satisfactorily the observed breakthrough curves of over 470 measured ASVs. A clustering analysis of the breakthrough curves was applied to establish a relation between the model parameters and bacteria physiology. The analysis showed that breakthrough curves form two clusters. One cluster was characterized by breakthrough curves with heavy tails and it was formed by small, motile, gram-negative bacteria. The other cluster displays strong peaks and a relatively weaker tailing. CTRW parameters are able to predict the cluster in which a certain ASV belongs.

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MS05 / 16

Experimental study of microbial hydrogen consumption rates by *Oleidesulfovibrio alaskensis* in porous media

Author: Raymond Mushabe¹

Co-authors: Nicole Dopffel ²; Na Liu ¹; Martin Fernø ¹; Geir Ersland ¹

¹ *University of Bergen*

² *NORCE*

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The recovery efficiency of short- and long-term cyclic operations of porous media underground hydrogen storage (UHS) is a key parameter for successful implementation, but anaerobic microbes autochthonous in the storage formation can consume hydrogen and adversely influence hydrogen recoverability and storage efficiency. Here we have experimentally measured hydrogen consumption rates by a model sulphate-reducing bacterium (*Oleidesulfovibrio alaskensis* G20) in drainage-storage cycles that mimic porous media UHS. Laboratory tests were performed in cylindrical sand pack columns as storage site analogues (inner diameter: 51.4 mm, length: 14.7 mm) with an average porosity of 28% at conditions of 37°C and 1.15 bara. The storage capacity (initial hydrogen saturation in place) of each sand pack was in addition analysed and compared against sterilized benchmarks. We observed an exponential decay in microbial hydrogen consumption between storage cycles: $28 \pm 12\%$ hydrogen was lost during the first cycle (with a peak average rate of $1.26 \pm 0.12 \mu\text{mol/hr/cm}^3$), compared with $10 \pm 5\%$ (second cycle) and $7 \pm 3\%$ (third cycle). The cumulative loss across the three cycles amounted to $15 \pm 6\%$, even though nutrient and carbon source concentrations were adequate for full hydrogen consumption in each cycle. The reduced microbial activity after the first storage cycle was explained by the observed increase in brine pH from initial 7.5 to 8.4 ± 0.2 at the end of the last storage cycle. We observed improvement in the average hydrogen in place saturations after the first non-sterile storage cycles. Our experimental data contributes to the understanding of microbial hydrogen loss during UHS and how it can affect the recovery and storage efficiency.

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MS04 / 17

Contact mechanics of soft grains considering capillary interactions

Authors: Jiayin Zhao¹; Haiyi Zhong^{None}

Co-author: Yixiang Gan ¹

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Granular soft materials (e.g., hydrogel spheres) have gained considerable attention due to their potential applications in drug delivery and tissue regeneration. To enable widespread applications of these materials in practical settings, it is crucial to accurately characterise the mechanical property (e.g., Young's modulus). Typically, the elastic properties can be determined through indentation tests. However, the formation of liquid bridges between the high-water-content surface and substrate introduces capillary forces, which adds complexities to contact mechanics and potentially compromises measurement accuracy. To address this, this study conducted indentation tests on

both single hydrogel, at different swelling stages, and rigid spheres to investigate the effects of capillary forces on force-displacement curves and stress distribution within the substrate. Experimental results showed strong agreement with a theoretical model for the cases of rigid spheres, while discrepancies were observed for hydrogel particles. These discrepancies, attributed to capillary forces, were analysed by measuring variations in liquid bridge curvature and the resulting local stress field, which were subsequently incorporated to refine the theoretical contact model. By isolating and accounting for the contribution of capillary forces, this study provides a reliable experimental method for accurately characterising the mechanical property of granular soft materials, ensuring their safe and effective use in various critical applications.

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Poster / 18

Semi-supervised Auto-segmentation Model for Enhanced Geomaterial Analysis

Author: Qinyi Tian¹

Co-author: Laura Dalton¹

¹ *Duke University*

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Understanding porosity in geomaterials is the critical first step to advancing applications like carbon capture and storage, enhanced geothermal systems, and hydrogen storage, where accurate modeling can improve storage efficiency, permeability calculations, and safety. Sandstone, known for its complex and highly porous structure, provides an excellent basis for testing and improving predictive models. In this work, we propose a semi-supervised model for efficient porosity calculation, aimed at reducing the reliance on extensive labeled datasets. Our approach builds on Geo-SegNet, our previously developed contrastive learning-enhanced U-Net model, which uses contrastive learning in the feature extraction process to improve porosity feature detection. By integrating both labeled and unlabeled data through a semi-supervised strategy and employing auto-segmentation for automated porosity feature identification, the model enhances data efficiency and scalability. This advancement offers a cost-effective and robust solution for geomaterial characterization, providing critical insights to support carbon storage efforts and improve our understanding of geomaterial behavior.

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MS01 / 19

Colloid-induced multiphase flow perturbations in porous media

Author: Muhammad Muqet Iqbal¹

Co-authors: Catherine Noiriél ; Cyprien Soullaine²; Sophie Roman³

¹ CNRS

² Stanford University

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Colloids in geological porous media such as rocks and soils are relevant for a broad range of environmental applications, such as groundwater remediation. The transport of colloids, ranging from nanometers to micrometers in size, is shaped by pore geometry, surface interactions, flow conditions, and particle properties [1]. In the literature, colloids are widely reported to influence the mobility of contaminants in porous media at the column scale [2], however, the multi-scale mechanisms driving colloid-induced mobilization, from microscopic interfaces to pore networks and field-scale processes, are poorly understood. This study addresses this gap using time-resolved 3D X-ray microtomography to investigate colloid transport, pore clogging, and flow modification under transient conditions.

By attaching to fluid interfaces, colloids can reduce capillary forces and aid non-aqueous phase liquids (NAPL) removal, while their deposition can clog pores and alter flow patterns [3]. Here we want to focus on modification in hydrodynamic forces due to pore clogging, which has already been evidenced by microfluidic experiments (as illustrated in figure 1b) [4]. Most of the previous studies at the continuum scale have focused on classical column experiments for colloid transport, missing the complex dynamics at the microscopic level. The existing pore scale studies either lack the third dimension (microfluidic experiments[5]), or in-situ imaging at sufficient spatio-temporal resolution to resolve the flow and transport [2]. To fill these knowledge gaps, this study aims to utilize X-ray microtomography that enables high-resolution, non-destructive imaging at the pore scale to investigate the mechanisms behind colloid-induced pore clogging, which modifies flow and mobilizes trapped NAPL in porous media [6]. Cylindrical samples of porous sintered glass (4 mm diameter, 40 mm length) with average pore throats in the range of 30–70 μm , are mounted in a flow cell (Figure 1a). To achieve our objectives, we conduct single-phase and multiphase flow experiments. We use three types of X-rays attenuating particles of varying sizes and surface properties to represent environmentally relevant colloids. This study is expected to provide insights into the role of colloids in pore clogging, and NAPL mobility.

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MS16 / 21

Pore-Fiber Transport Dynamics of Aqueous Cosolvent Solutions in Cellulose-based Thin Porous Media

Author: Sajjad Karimnejad¹

Co-authors: Elian Gonnet¹; Shuo Wang¹; Hamid Mansouri²; Nicolae Tomozeiu²; Anton A. Darhuber¹

¹ *Fluids & Flows Group, Department of Applied Physics, Eindhoven University of Technology,*

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After inkjet printing onto uncoated and unsized paper, the ink is first imbibed into the interfiber pores and subsequently absorbed by the cellulose fibers. The achievable print quality depends on the rate of this pore-fiber transport. The latter is accompanied by mechanical expansion of the fibers and the paper sheet. Therefore, we systematically monitored the swelling dynamics of several paper types as a function of ink composition by means of four different measurement techniques. Using aqueous cosolvent solutions as model inks, we found an approximately exponential relation of the time scales of porefiber transport with the cosolvent concentration and an approximately linear relation with its molecular weight.

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MS16 / 22

Long-term deformation of paper as a function of cosolvent mass transport in Latex Prints

Author: Jasper van den Hoek^{None}

Co-author: Ivo Schraven

Corresponding Authors: jasper.vandenhoeck@cpp.canon, ivo_schraven011@hotmail.com

Latex inks are one of the most prevalent types of inks within the inkjet printing market. These inks are water-based, but commonly contain cosolvents to tune their liquid properties. After the printing process these cosolvents are in part (<5 wt% cosolvents in paper) left in the paper, where over a period of days to months (long-term) they will redistribute to form a uniform concentration profile. This redistribution has been shown to correlate to long-term curl of prints on uncoated paper.[1] In this work, a model is proposed that describes the mass transport of cosolvents in paper by means of Fickian Diffusion, which is then coupled to a beam-bending model[2][3] to describe the evolution of paper curl over time.

The model is demonstrated to give a good fit to experimental results of different types of uncoated paper (sized and unsized paper). Herein the cosolvent concentration profiles were measured experimentally in an ex situ approach; print samples were sectioned to different thicknesses by a home-built milling apparatus after which the cosolvent concentration was determined by quantitative ¹H-NMR. In parallel, the deformation was measured also by a home-built device.

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MS24 / 24

Ab Initio Molecular Dynamics Investigation of Water and Butanone Adsorption on UiO-66 with Defects

Author: Brianne Boyd¹

Co-authors: Deep Choudhuri¹; Scott Bobbitt²

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Volatile organic compounds (VOCs) are harmful chemicals that are found in minute quantities in the atmosphere and are emitted from a variety of industrial and biological processes [1-3]. They can be harmful to breathe or serve as biomarkers for disease detection [4,5]. Therefore, capture and detection of VOCs is important. Here, we have examined if the Zr-based UiO-66 metal-organic framework (MOF) can be used to capture butanone - a well-known VOC. Toward that end, we have performed Born-Oppenheimer ab initio molecular dynamics (AIMD) at 300 and 500 K to probe the energetics and molecular interactions between butanone [CH₃C(O)CH₂CH₃] and open-cage Zr-UiO-66. Such interactions were systematically interrogated using three MOF structures: defective MOF with a missing 1,4-benzene-dicarboxylate linker and two H₂O; pristine MOF with two H₂O; and pristine dry MOF. These structures were loaded with one and four molecules of butanone to examine the effect of concentration as well. One-molecule loading interacted favorably with the defective structure at 300 K, only. In comparison, interactions with four-molecule loading were energetically favorable for all conditions. Persistent hydrogen bonds between the O atom of butanone, H₂O, and μ 3-OH hydroxyl attachments at Zr nodes substantially contributed to the intermolecular interactions. At higher loadings, butanone also showed a pronounced tendency to diffuse into the adjoining cages of Zr-UiO-66. The effect of such movement on interaction energies was rationalized using simple statistical mechanics-based models of interacting and noninteracting gases. Broadly, we learn that the presence of prior moisture within the interstitial cages of Zr-UiO-66 significantly impacts the adsorption behavior of butanone. Our findings are published in the journal *Langmuir*: <https://doi.org/10.1021/acs.langmuir.4c02502>.

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MS16 / 27

Transport of complex liquids in complex media as studied with NMR imaging

Author: Myrthe Reijnier¹

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To reduce its environmental impact, the printing industry is transitioning towards using water-based inks. The liquid vehicle typically contains, besides water, cosolvents and surfactants to modify the physical properties of the ink [1]. Pigments and polymeric particles are added to create the print itself. To optimize the print quality, a thorough understanding of the transport processes of these complex liquids in paper substrates is necessary. Most conducted research focuses on the uptake of liquid in uncoated cellulose sheets [2], [3], [4]. However, the effect of a coating layer, consisting of CaCO₃ and some polymeric binders, on top remains to be investigated.

Performing in-situ dynamic measurements of the imbibition process is challenging because the paper is only about 125 µm thin and the initial liquid uptake can be within 1 s [2]. Hence, large spatial and temporal resolutions are required. An ultra-fast NMR-based imaging technique [5], as schematically shown in figure 1, was developed for this purpose.

The transport mechanism is studied by following the obtained spatially dependent liquid distributions over time. An example of these liquid profiles obtained for the imbibition of a water-glycerol mixture, containing 20 wt% glycerol, can be seen in figure 2.

The results show that liquid imbibes without a clearly defined fluid front. Moreover, it is found that the short-term liquid uptake consists of three distinct phases which are different from the uptake in uncoated paper [3]. It is suggested that the coating acts as a resistance layer and slows down the imbibition such that imbibition and swelling happen at similar timescales.

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References:

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MS24 / 28

Molecular Insights into Caprock Integrity of Subsurface Hydrogen Storage: Perspective on Hydrogen-induced Swelling and Mechanical Response

Author: Mehdi Ghasemi¹

Co-author: Masoud Babaei¹

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The integrity of caprocks in subsurface hydrogen storage is crucial for preventing leakage and ensuring long-term safety. A significant yet often overlooked factor in caprock integrity is hydrogen-induced swelling in clay minerals. When hydrogen molecules are intercalated into the interlayer nano-space of clays, they can induce changes in the structural properties, such as the expansion or shrinkage of interlayer pores, which in turn can impact the mechanical response of the caprock. Using Molecular Dynamics simulations, we investigate how the intercalation of hydrogen within dry, partially to fully saturated of clay mineral interlayer spaces affect swelling behaviour and mechanical properties. In this talk, I will present our recent findings, providing new insights into the molecular mechanisms of this phenomenon and its implications for caprock integrity in subsurface hydrogen storage.

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MS24 / 29

Developing Effective Sorbents for Direct Air Capture using Large-scale DFT Calculations and ML Forcefields

Author: David Sholl¹

Co-authors: Andrew Medford²; Anuroop Sriram³; Logan Brabson²; Sihoon Choi²; Xiaohan Yu²

¹ *Oak Ridge National Laboratory*

² *Georgia Institute of Technology*

³ *Meta AI*

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Previous high-throughput computational modeling of crystalline sorbents relevant for Direct Air Capture (DAC) has typically relied on empirical forcefields (FFs), approximated sorbent structures as being rigid, and often considered only adsorption of CO₂. These assumptions are unlikely to be appropriate in developing practical DAC sorbents, which involve coadsorption of CO₂ and H₂O

in configurations that include chemical complexation and structural rearrangement of adsorbent microenvironments. To address these limitations, we have generated a data set with tens of millions of DFT calculations examining adsorption of CO₂ and/or H₂O in a diverse collection of metal-organic frameworks, including many materials with chemically-relevant point defects. This talk will discuss uses of this data set for directly identifying useful sorbents for DAC and also for developing machine learning FFs that can describe the full spectrum of adsorption in MOFs.

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Pore-scale study of an elongated bubble moving through a shear-thinning fluid

Author: Davide Picchi¹

Co-author: Pietro Poesio²

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The motion of elongated bubbles and ganglia in is frequently encountered in porous media. Although the study of confined bubbles is a canonical problem in fluid mechanics, a fundamental understanding of the problem is still an open issue when the fluids exhibit non-Newtonian behavior. Examples are biological solutions, emulsions, and polymers that behave like shear-thinning fluids, and their effective viscosity is a function of the imposed shear rate.

In this talk, we investigate the dynamics of elongated bubbles that move in an inelastic shear-thinning fluid that obeys the Carreau-Yasuda viscosity model by means of numerical simulations. We focus on regimes where inertia and buoyancy are negligible to assess the effect of the fluid rheology on bubble characteristics up to finite capillary numbers. First, we compare the results with the scaling laws obtained by lubrication theory by analyzing the trends of the film thickness and bubble speed. Then, we show the existence of a general scaling law for the effective viscosity that embeds both the zero-shear rate and shear-thinning effects and holds up to finite capillary numbers. Interestingly, the shape of the bubble is strongly influenced by the fluid rheology, which competes with the capillary number. Finally, the analysis of the viscosity fields shows an interplay between the zero-shear rate and shear thinning effects in different regions of the bubble, including the presence of recirculating vortexes that form ahead and behind the bubble.

These results clarify the effect of fluid rheology on bubble characteristics, and, although the motivation of our work is oriented toward understanding the dynamics of a single Taylor bubble, the scaling laws obtained may serve as a base for constructing more sophisticated models for trains of bubbles. We conclude by showing that the existence of a master curve for effective viscosity appears to be typical of a more general class of problems, including capillary imbibition (when a shear-thinning fluid invades a single pore) and flow in ducts with complex geometry.

Country:

Italy

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

Steinik, C., Picchi, D., Lavallo, G., Poesio, P., (2024). Capillary imbibition of shear-thinning fluids: From Lucas-Washburn to oscillatory regimes. *Physical Review Fluids*, 9, 023305 Barmak, I., Picchi, D., Gelfgat, A., Brauner, N., (2024). Flow of a shear-thinning fluid in a rectangular duct. *Physical Review Fluids* 9, 023303 Aquino, A., Picchi, D., Poesio, P., Dynamics of a Taylor bubble through a shear-thinning fluid up to finite capillary numbers, *Journal of Non-Newtonian Fluid Mechanics*, 105003, Picchi, D., Ullmann, A., Brauner, N., Poesio, P., (2021) Motion of a confined bubble in a shear-thinning liquid, *Journal of Fluid Mechanics*, 918, A7.

Poster / 31**Photons interactions with porous ink layer of a print and image output****Author:** Nicolae Tomozeiu¹**Co-authors:** Hamid Mansouri ; Helder Marques-Savaldor ²¹ Canon Production Printing B.V.² Canon Production Printing Netherlands**Corresponding Authors:** nicolae.tomozeiu@cpp.canon, hamid.mansouri@cpp.canon, helder.marquessalvador@cpp.canon

The latter developments in printing industry showed that the inkjet technology delivers good print quality using the flexibility of digital printing at a breakthrough cost price. At Canon Production Printing company, we consider the inkjet technology as the flagship of our successful R&D printer design and production.

The study of ink penetration in thin porous media (paper) is a challenging task and many results, mostly regarding the liquid transport, particle transport and paper deformation have been presented within this symposium in the previous editions. One special attention is paid in the last years to the outputs of a print process, namely image quality and print robustness. This means optical and mechanical properties of the thin ink layer onto porous paper.

In this work, we propose to reveal the main interactions of photons (especially in the UV-VIS optical domain) focusing on the color properties of the prints realized with water-based ink on porous paper. Theoretical models, experimental measurements and computational methods are proposed. The 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. High resolution - SEM is used to reveal the surface topography of the ink layer, as well as the presence of the voids of various dimensions into dried ink structure. The color computational methods take into accounts both structural and compositional properties of the print.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

MS15 / 32

Limitations of Deep Neural Network for Inversion Problems in Porous Materials: The Necessity of Mechanical Feature Integration

Author: Qinyi Tian¹

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As computational strength keeps growing, deep learning has emerged as a powerful technique for addressing complex tasks and solving problems with intricate logic. Researchers are starting to leverage deep learning methods to tackle all kinds of challenges, including inversion problems in different materials. However, training deep neural networks (DNNs) for such tasks requires extensive datasets, which may not always be available. In this work, we aim to utilize stress-strain curves to predict the microstructural features of the materials, but traditional DNN models alone demand substantial amounts of training data. To overcome the limitations of small datasets, we propose incorporating mechanical relationships as additional features within the model. By integrating domain-specific mechanical knowledge, our approach enables the DNN to learn effectively from limited data, enhancing feature extraction and prediction efficiency. This combined framework demonstrates how blending deep learning with physics-based constraints can improve performance and accelerate computations in data-scarce environments.

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Water & Porous Media Focused Abstracts:**References:**

MS06-A / 33

Performance of cyclic injections in soft granular media: Trapping efficiency and hysteretic behaviour

Author: Haiyi Zhong^{None}

Co-authors: Si Suo¹; Yixiang Gan²; Zhongzheng Wang³

¹ *Imperial College London*

² *The University of Sydney*

³ *Queensland University of Technology*

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Carbon dioxide (CO₂) and hydrogen (H₂) storage in geological formations are two key approaches to reducing carbon emissions, with capillary trapping being the most efficient mechanism for ensuring storage security. Understanding the behaviours of immiscible fluid-fluid displacement in porous media is crucial for optimizing trapping efficiency. Previous studies have primarily focused on trapping behaviours in fixed rigid particles during single injections, which may fail to accurately predict trapping efficiency. This limitation arises because storage media can be relatively deformable under pressures reaching MPa, and cyclic injections, rather than single injection, are commonly encountered in the field. This study experimentally investigates the effects of particle deformability (i.e., rigid and soft particles) on trapping behaviours during cyclic injections under quasi-2D conditions using a Hele-Shaw cell. Our results reveal significant differences in trapping behaviours between soft and rigid porous media. In soft porous media, gas bubbles evolve from cavities to ganglia, leading to a noticeable increase in residual saturation during cyclic injections. In contrast, rigid porous media exhibit initial pore invasion, with residual saturation remaining nearly unchanged throughout the cycles. Ultimately, soft porous media demonstrate higher storage capacity compared to rigid porous media. These findings provide valuable guidance for the development of more efficient geological gas storage strategies.

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References:

MS05 / 34

Biofilm Growth in Porous Media: A Radial-Flow Microfluidic Study

Author: Xuanyi Chen¹

Co-authors: Eoin Casey²; Dishon Hiebner²; Budi Zhao¹

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² *School of chemical and Bioprocess Engineering, , University College Dublin, Ireland*

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Abstract

Biofilms growth in porous media can significantly reduce permeability, influencing subsurface flow and transport processes relevant to groundwater remediation, waste containment, and enhanced oil

recovery. This study investigates biofilm development under radial flow conditions using custom-designed microfluidic chips. The chip design was simplified by incorporating axisymmetric radial flow with a heterogeneous pore size distribution, mimicking flow from a central injection point. *Pseudomonas fluorescens* biofilms were cultivated under varying flow rates using King's B medium, with time-lapse imaging monitored via a digital camera mounted on a microscope and injection pressure recorded using a pressure sensor. Results revealed permeability reductions of up to three orders of magnitude, depending on the injection flow rate. At low to moderate flow rates, higher injection rates promoted biofilm growth near the inlet, resulting in the higher permeability reduction. In contrast, higher flow rates produced uneven biofilm growth, localized clogging in non-dominant flow paths, and biofilm detachment, resulting in less pronounced permeability impacts. At the pore scale, biofilm growth predominantly initiated at channel intersections, with flow rates critically shaping spatial distribution. These findings illuminate the interplay between biofilm dynamics, hydraulic resistance, and nutrient gradients, offering insights to optimize biofilm-based applications for subsurface well injections.

Keywords: biofilm, porous media, Hydraulic Conductivity, Microfluidics, Bioclogging

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Water & Porous Media Focused Abstracts:

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MS06-B / 35

Modeling nanoparticle-stabilized foam flow in porous media accounting for particle retention and permeability reduction

Authors: Tatiana Danelon de Assis¹; Rouhi Farajzadeh²; Pavel Bedrikovetsky³; Grigori Chapiro⁴

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Nanotechnology has been rapidly growing in various industrial sectors, particularly in subsurface applications such as soil and aquifer remediation, greenhouse carbon storage, and enhanced oil recovery (EOR). An application of nanoparticles with great potential is the stabilization of emulsions and foams, which are used as mobility-control agents to optimize gas flooding. However, retention is a concern during the injection of suspended particles, as it can lead to reduced rock permeability and a decline in injectivity in injection wells. In the case of foam flow with nanoparticles, a high retention rate also reduces the number of particles available for foam stabilization, reducing foam flow efficiency. Consequently, conducting a quantitative analysis of nanoparticle loss is crucial for accurately evaluating foam stability. This work presents a model for nanoparticle-stabilized foam flow in porous media, accounting for particle retention and the resulting permeability reduction (Danelon et al., 2024c), based on the Stochastic Bubble Population model. We have included a transport equation incorporating suspended and retained nanoparticles based on the deep-bed filtration theory. We provide a semi-analytical solution under steady-state conditions, which allows

for obtaining water saturation, foam apparent viscosity, and pressure drop profiles. We study different nanoparticle concentrations (in the presence and absence of salt) using retention parameters based on experimental data. When particle retention is neglected, the sweep efficiency of the porous medium improves compared to the case without nanoparticles, even at a low nanoparticle concentration (0.1 wt%). In contrast, when retention is accounted for, this enhancement is observed only at higher concentrations (0.5 wt% and 1.0 wt%). The loss of suspended nanoparticles reduces their positive impact on the foam's apparent viscosity, while retained nanoparticles decrease permeability. Both effects increase water saturation, generally leading to a lower pressure drop compared to models that ignore retention. Nevertheless, the reduction in permeability directly increases the pressure drop, so whether the pressure drop increases or decreases when retention is considered depends on which of these opposing effects is dominant. Based on our findings, models that neglect nanoparticle retention and those that account for retention but neglect permeability changes underestimate the pressure drop, particularly in scenarios with significant retention (e.g., in the presence of NaCl and high nanoparticle concentration). Furthermore, we compared the semi-analytical steady-state solution with the dynamic solution for foam flow with nanoparticles (neglecting particle retention) proposed by Danelon et al. (2024a) and obtained an excellent agreement.

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Water & Porous Media Focused Abstracts:

References:

T. Danelon, P. Paz, G. Chapiro, The mathematical model and analysis of the nanoparticle-stabilized foam displacement, *Appl. Math. Model.* 125 (2024) 630–649. T. Danelon, R. Farajzadeh, P. Bedrikovetsky, G. Chapiro, Modeling nanoparticle-stabilized foam flow in porous media accounting for particle retention and permeability reduction, Under review (2024).

36

Shear-thinning Fluid Transport in Porous Media: Impact of Viscosity Ratio

Authors: Sina Omrani^{None}; Vahid Niasar¹

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Solute transport and mixing in heterogeneous porous media are critical to numerous practical applications. While most previous studies have focused on solute transport in the flow of Newtonian fluids, many processes involve this phenomenon in the flow of non-Newtonian fluids. In this study, a series of coreflooding experiments were conducted, supplemented by simulations, to compare the transport of xanthan gum (XG) as a shear-thinning fluid and water as a Newtonian fluid in porous media. Subsequently, the transport of miscible Newtonian fluids (NtoN) with a range of viscosity ratios (M) spanning from $\frac{1}{1000}$ to 1000 was analyzed in relatively homogeneous ($\sigma_{\ln k}^2 = 0.5$) and heterogeneous ($\sigma_{\ln k}^2 = 4$) porous media, with and without spatial correlation length. Furthermore, the transport of Newtonian fluids into shear-thinning fluids (NtoST) and vice versa (STtoN) was modeled in the same domains. The study investigates the impact of fluid rheology and the aforementioned parameters on solute transport, flow patterns, and dispersivity. The results reveal distinct behaviors in the influence of viscosity ratio during shear-thinning fluid flow compared to Newtonian fluid transport across various domains.

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MS09 / 37

Multiscale modelling of convection in porous media: experiments, pore-scale and Darcy simulations with dispersion**Authors:** Marco De Paoli¹; Howland Christopher J.²; Roberto Verzicco³; Detlef Lohse⁴¹ *Physics of Fluid Group, University of Twente & TU Wien, Institute of Fluid Mechanics and Heat Transfer*² *School of Mathematics and Statistics, University College Dublin*³ *Dipartimento di Ingegneria Industriale, University of Rome "Tor Vergata"*⁴ *Physics of Fluid Group, University of Twente***Corresponding Author:** marco.de.paoli@tuwien.ac.at

Convection in porous media is ubiquitous in natural and industrial processes. For mass transport in geophysical systems, solute dispersion is an important effect to be understood, and this dispersion cannot be described by molecular diffusion alone. The presence of solid obstacles in the porous matrix induces an additional solute spreading, due to the convoluted fluid movements through the medium. Modelling the dispersion effect remains a challenging task due to the vast parameter space encompassing medium properties such as porosity and permeability, fluid characteristics including buoyancy forces and diffusivity, and domain attributes like the height of the medium. As a result, multiple methods are required to understand the flow dynamics at the different scales involved, ranging from the level of the pores, with a sub-millimetre characteristic length, to the Darcy scale, involving hundreds of pores and relevant to practical applications. In this work, we investigate convection in porous media with dispersion using a combination of Hele-Shaw-like experiments in bead packs, pore-scale simulations and Darcy simulations. Building upon our previous work (De Paoli et al., *J. Fluid Mech.*, 987, A1, 2024), we present additional experimental results along with three-dimensional pore-scale simulations and Darcy simulations incorporating dispersion effects (De Paoli et al., SSRN, 2024). The mechanism of dispersion is accounted for by employing a Fickian anisotropic dispersion model (Wen et al., *Phys. Rev. Fluids*, 3, 12, 2018). The system considered is the Rayleigh-Taylor instability, consisting of two miscible fluids of different density in an unstable configuration, filling a saturated, homogeneous and isotropic porous medium. Results are compared in terms of global response parameters associated with the flow structure and mixing state of the system (namely, wavenumber, mixing length and mean scalar dissipation). In this well-defined and controlled configuration, we compare our findings to derive simple physical models and to identify suitable parameters to model the effect of dispersion at the Darcy scale.

This project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement MEDIA No. 101062123. We acknowledge the EuroHPC Joint Undertaking for awarding the project EHPC-REG-2023R03-178 access to the EuroHPC supercomputer Discoverer, hosted by Sofia Tech Park (Bulgaria).

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References:

De Paoli, M., Howland, C. J., Verzicco, R., & Lohse, D. (2024). Towards the understanding of convective dissolution in confined porous media: thin bead pack experiments, two-dimensional direct numerical simulations and physical models. *Journal of Fluid Mechanics*, 987, A1. Wen, B., Chang, K. W., & Hesse, M. A. (2018). Rayleigh-Darcy convection with hydrodynamic dispersion. *Physical Review Fluids*, 3(12), 123801. De Paoli, M., Yerragolam, G. S., Lohse, D., & Verzicco, R. AFiD-Darcy: A finite difference solver for numerical simulations of convective porous media flows. Available at SSRN 4995113.

MS08 / 40

Evaluating the uncertainty of upscaled reaction rates in a structured fluvial aquifer using an ensemble mass transfer particle tracking framework

Author: Nick Engdahl¹

¹ *Washington State University*

Corresponding Author: nick.engdahl@wsu.edu

Mixing limited reactions are highly influenced by the architecture of the geological deposits they flow through because the structured nature of the material can severely limit the ability of the reactants to mix. The complex patterns created by meandering and braided rivers result in sharp interfaces that interrupt correlation lengths and directions that are below the typical resolution of simulation grids for field scale problems. How to accurately upscale their effects without explicitly resolving these sedimentary contacts is unclear, meaning that predictions of reactive transport behaviors in such systems remain highly uncertain. This work investigates how these small scale (<1m) sedimentary structures affect local and global mass transformation rates for a mixing limited reaction system. A hybrid Lagrangian method, termed mass transfer particle tracking (MTPT), was used to resolve the small-scale mixing processes as realistically as possible at the centimeter-scale representative elementary volume size for these deposits. An ensemble of over 250 highly conditioned realizations of the hydrogeology of a 16m by 4m by 3.5m study site along the Rio Grande in Albuquerque, New Mexico were used along with the MTPT framework to quantify the uncertainty in the reaction rates over time. The ensemble results were then compared to the amount of mass that would be produced if each domain were homogenized instead. Using the average resulted in higher times more mass production than the ensemble and the variance of homogenized simulations exhibited a much larger range of rates. Accounting for this difference could allow more robust representations of reaction rates in models that do not explicitly include the small-scale geological contacts, so several upscaled models for doing based on the geological structure are considered for steady-state and transient reactive transport scenarios. We show that reactant covariance- or colocation-based models are highly accurate as descriptive tools and present evidence that they show strong potential as predictive tools as well.

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References:

41

Molecular Dynamics Simulation of the Effect of Salt Type and Brine Salinity on the Wetting Properties of Hydrogen-Brine-Calcite System

Author: Yasaman Haghighatnejad¹

Co-authors: Hassan Mahani ¹; Nahid Pour Khiabani ¹; Shahab Ayatollahi ¹; Mohammad Amin Esmaeilbeig ²

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Underground hydrogen storage (UHS) has emerged as a promising solution for energy sustainability. The wettability behavior of hydrogen in contact with brines and mineral surfaces plays a pivotal role in hydrogen storage and withdrawal. Therefore, understanding the governing factors is critical for maximizing storage capacity and the hydrogen recovery factor. Molecular dynamics (MD) simulations were employed to investigate the impact of brine composition (NaCl and KCl) and concentration on the wettability of the 101 $\bar{4}$ calcite plane in the presence of hydrogen. The simulations were conducted at temperature of 373 K, pressure of 250 bar, and 0.1 and 1 M salt concentrations. To gain a deep understanding of the results, radial distribution functions, potential energy, and density profiles were determined. We found that regardless of the brine salinity and cation type, the contact angle of a water droplet in the presence of hydrogen on a smooth calcite surface represents a strongly water-wet system, resulting in the spreading of water and formation of a stable water layer. However, the distribution of hydrogen near the calcite surface is notably influenced by both the brine composition and salinity which would alter the wettability over a long time or affect the hydrogen-calcite geochemical reactions. It was observed that, at 0.1 M salinity, hydrogen molecules distribute in the solution with distances higher than 4 Å from the calcite surface, while at higher salinities, they stay away from the solid surface, facilitating increased water accumulation at the solid-liquid interface. In other words, more hydrogen is retained in the gas-water interface for more concentrated brines. In NaCl solutions, hydrogen molecules are located closer to the solid surface, at an average distance of 7 Å, whereas in KCl solutions, they are pushed farther away, approximately 12 Å above the surface. The results of this study could help the optimal selection of underground hydrogen storage reservoirs through molecular simulations.

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Water & Porous Media Focused Abstracts:**References:**

MS08 / 42

Impact of hydrodynamics on accessible mineral surface area

Author: Lauren Beckingham¹**Co-author:** Cyprien Soullaine²¹ *Auburn University*² *CNRS***Corresponding Authors:** cyprien.soullaine@gmail.com, leb0071@auburn.edu

Predicting mineral reaction rates in porous media is challenging, in part due to the difficulty of accurately quantifying mineral reactive surface area. Mineral accessible surface area, the surface area of mineral phases in contact with reactive fluids, is an improved means of estimating mineral reactive surface area in multi-mineralic systems. Accessible mineral surface areas can be obtained from multi-scale imaging analysis and integrated into reactive transport simulations. However, variations in hydrodynamics at the pore scale may restrict the interaction of accessible mineral surfaces with the reactive fluid. Here, we aim to characterize the impact of hydrodynamics on mineral accessibility for varied flow conditions using direct numerical simulations carried out in OpenFOAM. A series of simulations considering transport of a solute through varied porous media domains, from simple to more complex geometries, are carried out considering a range of typical flow conditions captured by varied Peclet numbers. For each simulation, the impact of hydrodynamics on mineral reactivity is considered by tracking the evolution of the solute concentration at the particle surfaces over time. Simulation results reveal the conditions under which hydrodynamics must be considered to accurately capture mineral reactivity.

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MS06-A / 43

Impact of inertia and wetting films on the stability of two-phase flow: a pore-doublet approach

Authors: Nathan Bernard¹; Cyprien Soullaine²; Sophie Roman³¹ *CNRS*² *Stanford University*³ *University of Orleans***Corresponding Authors:** nathan.bernard@cnrs-orleans.fr, sophie.roman@univ-orleans.fr, cyprien.soullaine@gmail.com

Accurately predicting multiphase flow is a challenging task because the displacement of the two fluid phases depends on a complex interplay between surface tension effects and viscous forces, resulting in non-linear behavior. In this study, we employ pore-doublet models to investigate the

stability of two-phase flow across a wide range of fluid properties and flow rates. Pore-doublers –a conceptual model consisting of two parallel pores –are commonly used to explore two-phase flow stability in porous media. We develop a novel dynamic pore-doubler model with identical channels that incorporates the effects of inertia and Bretherton’s films—factors often neglected in pore-doubler modeling. Direct comparisons between the model and microfluidic experiments reveal that both inertia and Bretherton’s films significantly influence the stability of the invasion process. We demonstrate that including these effects in the model is crucial for achieving accurate predictions of flow regimes. Finally, we show that pore-doubler models with wetting layers can replicate stability phase diagrams similar to the Lenormand phase diagrams, despite the latter being derived from complex porous structures.

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MS09 / 44

Influence of particle shape on packing structure and non-linear hydraulic behavior

Author: Jike Li^{None}

Co-authors: Deheng Wei¹; Yixiang Gan¹

¹ *The University of Sydney*

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Granular media, exhibiting permeable packing structures, commonly exists in various fields of civil engineering, ranging from soil drainage, oil and gas extraction, to mining, and underground gas storage. The packing structure is dominated by grain features, such as size distributions, general shapes, and fine morphology features. Due to the opaque nature of overwhelming parts of natural grains, instant changes of the porosity and tortuosity reflected by pore geometry are hard to quantify experimentally. To bridge this gap, this numerical study is twofold: i) systematic investigations on influences of initial grain shapes on the fabric tensor during compaction process, and ii) the resultant hydraulic conductivity in transition flow. The first point is accomplished using the discrete element method (DEM), while the latter is conducted by solving Reynolds-Averaged Navier-Stokes (RANS) equations at pore-scale. In this study, DEM can quickly and accurately assemble packing structures consist of mono-dispersed grains in natural shape; meanwhile, the fabric tensor in each assembly is computed from the resulting packing structure. Realistic shaped grains, generated using the inverse analysis of Spherical Harmonics, are imported into DEM for the assembly, in order to systematically study the grain shape effects. The results indicate that the grain rearrangement and deformation from the compaction process could decrease porosity, introduce anisotropic features, and increase the global pore tortuosity, and therefore suppress the permeability. Our findings will contribute to the understanding of effects of grain shapes and compaction on permeability, beneficial to the engineering applications concerning the fluid flow in various types of porous materials.

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MS11 / 45

New progressive particle clogging mechanism by dendritic build-up in porous domains.

Author: Walid OKAYBI^{None}

Co-authors: Cyprien SOULAIN ; Sophie ROMAN

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Understanding the transport and deposition of colloidal particles in confined environments is crucial for optimizing natural and engineered systems, such as groundwater remediation and filtration technologies. This study adopts a pore-scale approach, combining microfluidic devices that mimic rock structures with pore-scale flow simulations to investigate clogging mechanisms, uncovering a unique phenomenon termed dendrite clogging. Unlike traditional progressive clogging, dendrite clogging arises from particle buildup at a single deposition site—the dendrite tip—which extends toward adjacent grains to block pathways. We experimentally confirm that dendritic structure formation is highly flow-rate dependent, identifying a critical velocity threshold (V_c), derived from drag-adhesive torque balance, beyond which particle attachment is suppressed. When normalized flow velocity (V_f / V_c) is less than 1, cone-shaped stagnation zones form, enabling particle attachment. Experiments on single-grain collectors validate this criterion, showing dendritic structures when stagnation zones accommodate particles along the collector's centerline. Increasing flow rates compress these zones, limiting attachment. Applying this criterion to porous domains reveals that dendrite formation depends on the accommodation capacity of stagnation zones. We demonstrate that flow behavior is significantly impacted by particle deposition and clogging, as evidenced by the observed increase in experimental and simulated pressure differences alongside porosity decline with increasing pore volumes injected. Interestingly, this trend stabilizes over time, suggesting that fluid velocity eventually surpasses the critical threshold for particle attachment. These findings provide insights into the formation of unique clogging mechanisms by dendrites in porous domains, with practical implications for improving the performance and efficiency of porous systems.

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References:

MS13 / 46

Tuning the wetting properties of micro- and meso-porous carbons: nanoscale insights from time-resolved synchrotron SAXS

Author: François Chaltin¹

Co-author: Cédric Gommès²

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In many applications, such as catalysis, electrochemistry or fuel cell, the performance of nanoporous materials hinges on their ability to retain or repel liquid within their porous structure. A critical challenge in these applications is determining whether this liquid distribution is uniform or whether certain pores remain inaccessible. Macroscale wetting phenomena are well-explained by energy considerations of wet versus dry surfaces, but this understanding does not easily extend to the nanoscale. At molecular dimensions, the applicability of traditional physical models becomes uncertain. The complex architecture of nanoporous materials, with diverse pore sizes and intricate connectivity, further complicates the analysis. Beyond equilibrium aspects of spontaneous pore infiltration, understanding the kinetics of liquid penetration in relation to pore permeability, introduces additional challenges.

Here, we investigate wetting dynamics in carbon xerogels, which materials are characterized by a dual-pore system comprising mesopores (~20 nm) and micropores of near-molecular dimensions (< 2 nm). By performing capillary-rise experiments with water and employing synchrotron Small Angle X-ray Scattering (SAXS), we gained time- and space-resolved insights into the wetting mechanisms at nanoscale. Different xerogels were studied to assess the influence of structural variations, including conditions where micropores were pre-saturated via water vapor adsorption, and oxidized samples with altered surface energy. All experiments were conducted at the Belgian DUBBLE beamline (BM26) at the European Synchrotron Radiation Facility.

We recently highlighted a two-step wetting process, with an early filling of molecular-sized micropores followed by the later filling of the mesopores. A Cassie-Baxter analysis of our results demonstrates that initial micropore wetting dramatically alters the surface properties of adjacent mesopores, turning them from hydrophobic to hydrophilic. Surprisingly, experiments with oxidized carbon xerogels, designed to enhance hydrophilicity, revealed faster capillary rise in mesopores but restricted water infiltration into the micropores. This unexpected finding, which will be presented for the first time, highlights the role of surface chemistry in modulating nanopore accessibility and challenges conventional assumptions about hydrophilicity-driven wetting enhancement.

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References:

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47

Improved Oil Recovery Through Unstable Injection and Production: A Case Study on Mature Oilfield in Kazakhstan

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Mature oilfields are facing the problem of interlayer interference led by long-term general water injection, as well as the unfavorable deployment of new wells due to large well density. Unstable Injection and Production is a cost-efficient way to improve oil recovery, which includes the concept of separate-layer injection-production and cyclic injection-production. This paper proposes 4 unstable injection-production well recombination pattern: separate-layer production and injection (SPSI), separate-layer production and cyclic injection (SPCI), cyclic production and separate-layer injection (CPSI) and cyclic production and injection (CPCI), take the K field in Kazakhstan as an example, studies the effects of different patterns and cycles on the oil recovery using numerical simulation method. The conclusions are presented as follow: 1) Unstable Injection and production can improve oil recovery in a short period of time, SPCI has the best result of improving oil recovery under the research condition; 2) Under the same working schedule of oil wells, the effect of cyclic injection is better than separate-layer injection; 3) Under the same working schedule of water injection wells, the effect of separate-layer production is better than cyclic production; 4) With the shortening of the alternate cycle, the effect of SPCI on IOR becomes worse first and then better; 5) The shorter the alternate cycle, the better the effect of CPSI on IOR; 6) The shorter the alternate cycle, the better the effect of CPCI on IOR. This research has certain guiding significance for improving oil recovery and production-injection optimization of mature oilfields.

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References:

MS20 / 48

Understanding thermoregulation and ventilation in termite mounds for eco-friendly building solutions

Authors: Nengi Karibi-Botoye¹; Guy Theraulaz²; Bagus Muljadi³; Julien Maes⁴; Hannah Menke⁴; Vasily Demyanov⁵; Kamaljit Singh⁴

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Termite mounds are renowned for their ability to maintain self-sustained ventilation and thermoregulation irrespective of external climatic conditions. Although there has been significant interest in this topic, especially for designing energy-efficient buildings, it is still unclear how the mound properties are controlled. In this study, we combine X-ray tomography and numerical simulations to correlate structural properties and function in mounds constructed by *Trinervitmes geminatus*, *Cubitermes*, *Apicotermes* and *Thoracotermes* termites species. The results show a variation in flow and thermal properties in the different mounds. We find that the fluid flow in the mound is strongly controlled by the outer wall properties. We also observe that structural properties of the mound like macroporosity as well as microporosity play a crucial role in determining the diffusion of heat and CO₂ through the structure. These results will be integrated with findings from other species obtained from in-situ measurements and mounds scanned at microscale, allowing us to gain a deeper understanding of the processes governing self-sustained ventilation and thermoregulation in termite mounds.

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Water & Porous Media Focused Abstracts:

References:

MS06-B / 49

Pore-Scale Modelling and Simulation of Precipitation and Crystallization in Porous Media: Insights into Clogging Patterns for CO₂ Mineral Trapping

Authors: Sarah Perez¹; Jean-Matthieu Etancelin²; Andreas Busch¹; Philippe Poncet²

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Understanding reactive microscale flows in porous media is essential for managing the geochemical processes involved in subsurface CO₂ storage. These processes, including precipitation, crystallization, and dissolution, contribute to the mineral trapping of injected CO₂ and govern the evolution of fluid-mineral interfaces. Bridging these pore-scale phenomena with their large-scale implications is

critical for assessing storage capacity and ensuring reservoir integrity, thereby facilitating effective risk management of CO₂ storage sites.

This work explores the numerical simulation of precipitation and crystallization in realistic porous media geometries obtained by X-ray microtomography. By coupling superficial velocity models with a Lagrangian formulation of the chemistry, the method achieves a high degree of efficiency and accuracy in simulating reactive flows at the pore scale.

We introduce a two-step crystallization model for CO₂ mineral trapping, which includes the primary homogeneous nucleation of the dissolved chemical species and crystal growth driven by interactions with the solid interface. The model incorporates a probabilistic reaction rate for the crystal growth, accounting for the geometrical dependency in the aggregation of the precipitate at the interfaces. This approach enables the investigation of flow path restructuring caused by partial or complete clogging of pore throats. This will ultimately impact the prediction of flow and transport in CO₂ storage reservoirs.

Numerical simulations reveal distinct clogging and non-clogging regimes, highlighting the importance of both geometrical features and flow parameters in pore-scale mineral trapping. To further characterize these phenomena, we propose an additional dimensionless number that contributes to the identification of clogging patterns based on the adsorption frequency of the precipitates to the mineral interface. Finally, the impact of these microscale interfacial phenomena on macroscale porosity and permeability is investigated across different regimes, with comparisons between clogging and non-clogging configurations.

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Water & Porous Media Focused Abstracts:

References:

MS23 / 50

Geology and Petrophysics of US Natural Gas Storage Reservoirs and Caprocks with respect to Suitability for Hydrogen Storage

Author: Franek Hasiuk¹

¹ Sandia National Laboratories

Corresponding Author: fhasiu@sandia.gov

The Hydrogen Economy is one proposed model for decarbonizing the hydrocarbon industry while still utilizing much of its infrastructure. One anchor of our current hydrocarbon industry in the US and Canada is the fleet of 635 porous media and salt cavern facilities where natural gas is stored on a seasonal cycle. Because the energy per unit volume of hydrogen is approximately one-third of natural gas, a Hydrogen Economy would need approximately three times as much pore space to accommodate the current amount of energy stored. This would likely require a mix of expansion at some current facilities as well as the construction of new storage facilities. In light of this potential need for re-evaluation of current facilities and exploration for new facilities, a database was built of all currently operating natural gas storage facilities as well as closed facilities for which some record exists

publicly. For each facility, the age, formation, and lithology of the reservoir and caprock were identified for each storage unit in a facility (i.e., some facilities have multiple reservoirs). The trap type (e.g., structural or stratigraphic) was noted. In total, 715 reservoir-caprock pairs were identified in the US and Canada. The most common reservoir type was a Devonian/Mississippian/Pennsylvanian sandstone depleted petroleum reservoir (n=251). The next most common was a Silurian carbonate petroleum reservoir (n=47), followed by Jurassic salt caverns (n=42). Reservoir lithology was geographically dependent. For example, in the West and Alaska most reservoirs were Cretaceous or Paleogene in age, while in the rest of the country they were Paleozoic in Age. Salt storage is only found on the Gulf Coast. Work is ongoing to identify type petrophysical well logs for each facility and build a database of petrophysical properties (e.g., porosity, permeability) that can be used for geological modeling and reservoir simulation of hydrogen storage in these and potential greenfield sites.

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References:

MS25 / 51

In-situ observation of mafic/ultramafic rock reactions with supercritical CO₂ using neutron reflectometry

Authors: Candice Halbert¹; Chelsea Neil²; Chris Keeter¹; Christopher Neal¹; Erik Watkins¹; Hari Viswanathan²; Jim Browning¹

¹ Oak Ridge National Laboratory

² Los Alamos National Laboratory

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Fast carbon dioxide (CO₂) mineralization has been recently observed in mafic and ultramafic rocks, promoting CO₂ stabilization and reducing risky reliance on caprock integrity. However, there are currently many unknowns surrounding these new observations, including reaction kinetics for different minerals. In the current study, we apply neutron reflectometry (NR) to make in situ observations of the fluid-rock interface to characterize these geochemical interactions for olivine, serpentine, and basalt thin films. We observed minimal reactivity for basalt compared with ultramafic minerals. Surprising, more alteration of serpentine was observed than olivine, despite reported lower reactivities. Through this work, we can advance our understanding of dissolution and secondary mineral precipitation during GCS in mafic/ultramafic rocks, which will allow optimization of CO₂ mineralization through improved site selection and more accurate geochemical modeling.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

MS07 / 52

Pore-Scale Modeling and Relative Permeability Upscaling in Stress-Sensitive Fractured Porous Media

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Co-author: Marcio Murad²

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² *Laboratorio Nacional de Computacao Cientifica*

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We investigate multiphase flow in rough-walled fractures within stress-sensitive rocks, addressing the complexities introduced by rock deformation and fracture geometry. At the pore scale, we employ a Lattice-Boltzmann formulation to simulate flow under various conditions, parametrized by fracture aperture, joint roughness coefficient (JRC), contact angle, and viscosity ratio. The simulations capture detailed physical processes at the fracture scale, enabling the generation of a family of relative permeability curves. These curves deviate significantly from traditional correlations for 3D porous media, reflecting the unique dynamics of flow in fractured systems. Through an upscaling process, we derive robust parametrization for the relative permeability curves. Additionally, we explore the Barton-Bandis law, which models the hyperbolic relationship between normal stress and fracture closure, to examine the effective stress influence upon the flow patterns. Perturbation analyses reveal stress-induced variations in the relative permeability curves, highlighting their sensitivity to mechanical deformation. To extend these insights to larger scales, we consider an idealized fracture arrangement within a coarse computational cell and perform steady-state, flow-based upscaling. This approach yields homogenized macroscopic relative permeability curves that capture the interplay between capillary forces and viscosity contrasts across various regimes. The proposed methodology provides a framework for analyzing the stress-sensitive behavior of these curves under realistic geological conditions. Finally, numerical simulations demonstrate the predictive capability and versatility of the model in capturing complex multiphase flow phenomena in fractured, stress-sensitive rocks. These results underscore the importance of incorporating fracture mechanics and detailed pore-scale physics into macroscopic flow models for improved characterization of fractured reservoirs.

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Poster / 53

Investigating hydrogen behavior in shale nanopores using small-angle neutron scattering

Authors: Chelsea Neil¹; Hyeonseok Lee¹; Lilin He²; Michael Gross¹; Mohamed Mehana^{None}; Tim Germann¹

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Hydrogen behavior in tight rock formations will define the success of many subsurface operations, including geologic hydrogen production and seasonal storage. Understanding the fundamental mechanisms governing transport within these systems necessitates the application of advanced experimental techniques capable of nanoscale observation under dynamic and high-pressure conditions. In the current study, we demonstrate the powerful and unique capability of small-angle neutron scattering (SANS), when combined with pressure cells, to provide insight into hydrogen behavior in shale nanopores. Results shed new light on the links between pore fluid chemistry and hydrogen gas trapping, as well as quantification recovery during pressure cycling.

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References:

MS11 / 54

Coupling microfluidics and Raman spectroscopy to measure concentration gradients in geological porous media

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Most of the world's drinking water supply comes from groundwater aquifers. These sources, however, are susceptible to contamination (hydrocarbon, chlorinated solvents, nitrates...). Environmental engineering applications foreseen the usage of charged colloidal particles for groundwater remediation or for sealing damaged geological confinement barriers. However, the injection of colloidal particles into the area of interest in a geological formation using conventional mechanisms such as pressure gradients or gravity is challenging. Using solute concentration gradients, it is possible to induce the particles to flow into or out of the pores under controlled conditions. This phenomenon

is known as diffusiophoresis. In geological porous media, local concentration gradients arise from a number of physico-chemical processes such as salt or crystal dissolution, drying, precipitation, interphase mass transfer, chemical reactions, and can lead to diffusiophoretic transport of colloidal particles. The present study assesses the magnitude and spatial distribution of local concentration gradients generated in situ during the dissolution of calcite crystals, and evaluate their potential to deliver colloidal particles to regions of interest.

We developed an approach that combines microfluidic devices with Raman spectroscopy, a non-invasive, non-destructive technique that allows the in situ identification of chemical species and their transformation during a reaction [1]. We perform Raman spectroscopy in real time during calcite dissolution under dynamic conditions. From Raman spectra we obtain the calcite and solute compositions, thus providing new insights into hydro-geochemical coupling in porous media. The experimental results will extend the numerical models developed that simulates the dissolution of calcite at the pore-scale [2]. In a second step, more complex reactive micromodels will be considered, like flow-through reactors to localize concentration gradients generated by dissolution/precipitation. The anticipated outcomes aim to contribute significantly to the understanding of local concentration gradients in geological porous media, paving the way for improved predictions and management of subsurface processes.

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2

55

Investigation of the influence of viscosity ratio on oil clusters mobilization in Tertiary EOR-like microfluidic experiments

Author: Haohang Pi^{None}

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In this work we experimentally investigate the enhancement of tertiary oil recovery by injection of viscous fluids. Experiments were performed on 2D water-wet microfluidic chip of irregular structure and viscous fluids were Glycerol/water mixture of various composition. Fluids were fed to the chip under controlled flow rates while acquiring images at large and pore scale by means of a CCD camera

mounted on an optical microscope. Also, all fluids were dyed so that after the image processing step, it was possible to make distinction between all present phases. Our work encompasses the study of the usual drainage and imbibition steps before starting injection of Glycerol/water mixtures. However, we particularly focus on characterising mechanisms by which additional oil is produced when such mixtures are injected after the waterflooding step. We were mainly interested in the change of oil clusters location in the porous medium and their becoming when the viscosity of injected mixture is increased. We show therefore that as the number of oil-filled pores decreases by increasing the mixture's viscosity and the additional oil recovery that initially start by sweeping large pores is progressively shifted to smaller pores. This was also evidenced as the size distribution of oil-filled pores is more and more biased toward smallest pores for higher viscosity. To investigate the oil clusters becoming they were categorized in class of ganglia, blobs and droplets and both their number density and volume were followed in the course of time for each injected mixture. From these data, and given our experimental conditions, we put forward that the oil clusters removal mechanism may be phenomenologically described as follows:

Right after the water flooding period and before mixture injection, oil clusters remain integer and immobile throughout the chip. Once the mixture is introduced at the same flow rate, it first replaces water upstream, then flows preferentially along pre-existing waterflooding pathways, displacing water and gradually increasing pressure within the chip. This pressure build-up rapidly stresses the clusters, breaking them into smaller droplets and blobs, which are subsequently transported. The elevated pressure also mobilizes and redistributes downstream clusters, altering their size and location. As injection progresses and more areas of the chip are swept, further ganglia breakup occurs, with the fragments carried away by the mixture. In this picture and as it is schematically illustrated in the attached figure, the characteristic time for ganglia breakup is shorter than that for small oil fragments transport, enabling efficient mobilization. Overall, oil cluster evolution before mixture breakthrough is dynamic and is related to local change of fluid composition and flow structure in a cascading pressure build-up, local increase of stress, oil clusters breakage and mobilization and transport

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References:

MS01 / 56

Hydro-Geomechanical Reservoir Modelling of Underground Hydrogen Storage in a Saline Aquifer of the North German Basin

Author: Anna-Maria Eckel¹

Co-authors: Lea Döpp¹; María Belén Febbo¹; Mrityunjay Singh¹; Cornelia Schmidt-Hattenberger¹

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To balance the seasonal fluctuations of supply and demand in renewable energy, hydrogen can be produced using excess electricity and temporarily stored in geological formations. Due to their large storage capacities and widespread distribution in sedimentary basins, saline aquifers have great potential for underground hydrogen storage (UHS). However, the practical feasibility of UHS in porous

formations remains to be demonstrated. This study focuses on the Triassic Stuttgart Formation near the city of Ketzin, a site located in the North German Basin previously used for a carbon dioxide (CO₂) storage pilot project. The formation is lithologically heterogeneous and its anticlinal structure offers potential as a structural trap for hydrogen storage. However, the presence of a fault zone at the top of the reservoir raises concerns about potential gas migration, which could be intensified by the geomechanical effects induced by cyclic hydrogen injection, thereby compromising the integrity of both the reservoir and the caprock.

Previous UHS modelling efforts on the reservoir scale have predominantly focused only on hydrodynamic aspects, while the geomechanical effects in geological porous media remain underexplored. However, their understanding is critical for ensuring safe, long-term hydrogen storage. To address this gap, this study presents a coupled hydro-geomechanical reservoir model to evaluate key geomechanical phenomena such as reservoir fracturing and the reactivation of faults. Numerical reservoir simulations are conducted using site-specific field data and performed using the computational simulator software CMG GEM. The output is assessed under varying operational scenarios (e.g., change of injection and production pressure).

The results provide critical insights into the flow and geomechanical behaviour of UHS operations in a saline aquifer of the North German Basin. Even though this analysis is site-specific, it strongly enhances understanding of the mechanical integrity of the reservoir and caprock, contributing to the broader development of hydrogen storage technologies in saline aquifers. Ultimately, the findings will advance the study of the feasibility of UHS and additionally support the design and evaluation of a prospective hydrogen storage demonstrator.

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References:

MS01 / 57

Numerically predicting surface displacement patterns to inform monitoring well strategies in underground H₂ storage for a reservoir at Ketzin site in Germany

Author: Mrityunjay Singh¹

Co-authors: Cornelia Schmidt-Hattenberger ¹; Ben Norden ¹; Ingo Sass ¹

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The transition to a sustainable energy landscape has intensified interest in geological storage of hydrogen (H₂) as an energy carrier and buffer. Repeated injection and withdrawal of H₂ induce complex thermo-poroelastic responses in the subsurface, making it essential to predict these changes accurately to ensure reservoir integrity and informed reservoir management. This study employs a coupled thermo-poroelastic finite element model built within COMSOL Multiphysics to simulate the geomechanical and thermal evolution of a reservoir at the Ketzin site in the North German Basin, Germany, during H₂ injection and extraction phases. The model incorporates fluid flow, heat transport, and mechanical deformation in a fully coupled manner. By doing so, it provides realistic

estimates of pore pressure variations, temperature gradients, and resulting stress field alterations. A key focus of the simulations is quantifying the spatial and temporal distribution of surface displacement near the operational wellbore for a given injection scenario. Near the injection wellbore, pressure-driven flow maintains higher gas saturations, whereas further away from the wellbore, plume spreading leads to lower saturation levels. These reservoir dynamics translate into subtle yet detectable deformation patterns at the surface. Thermo-hydro-mechanical coupling significantly influences porosity and permeability changes during cyclic operation, while thermoelastic effects remain relatively small due to limited temperature contrasts between injection fluids and the reservoir. The fully coupled thermo-poroelastic changes can lead to vertical displacement on the order of millimeters, potentially accumulating over multiple cycles and affecting the near-surface stability and infrastructure, however it remain very small.

One key finding is that localized uplift signals evolving over the injection-withdrawal cycle serve as diagnostic indicators of subsurface stress distribution and fluid fronts. Leveraging these insights, we investigate optimal placement strategies for a dedicated monitoring well. By positioning this well at a strategically chosen offset from the operational wellbore, it becomes possible to directly measure critical parameters such as pressure, temperature, and deformation, while minimizing operational risks and maximizing the value of collected data. Such monitoring can capture early signs of fluid migration and mechanical response, thereby supporting proactive reservoir management and early warning detection systems.

Beyond the exemplary Ketzin case, the modeling framework and insights presented here can be extended to other subsurface hydrogen storage sites worldwide in sedimentary basins. By linking geomechanical simulations to practical monitoring strategies, this research advances the reliable, safe, and efficient long-term storage of hydrogen in the pursuit of a more sustainable global energy future.

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Poster / 58

Determining Tracer Dispersion Properties in Porous Media Using the Galerkin Physics-Informed Neural Network Approach

Author: Luis Constante¹

Co-authors: Adolfo Pires¹; MARTIN A. DIAZ-VIERA²; Jesús M. Carmona-Pérez³

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This study addresses the challenge of modeling tracer dispersion through porous media, applying the Galerkin Physics-Informed Neural Network (Galerkin PINN) approach. The Galerkin PINN method has been systematically evaluated by comparing its results against both analytical solutions and numerical simulations using a Finite Element Method. In this work, experiments were conducted using Berea sandstone, a representative natural porous medium, to validate the model's accuracy in real-world scenarios. A significant aspect of this research involved solving the inverse problem to

accurately determine the dispersion coefficient, which is crucial for predicting the behavior of tracers in geophysical and environmental engineering applications. The numerical results demonstrate that the Galerkin PINN approach not only reproduces precisely the empirical data but also offers an efficient alternative since shows an improvement in computational performance and adaptability, making it a promising tool for complex flow and transport problems in heterogeneous porous media.

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MS05 / 59

Pore-scale bio-geochemical reactions and their impact on reservoir properties in underground hydrogen storage

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A significant barrier to underground hydrogen storage is that hydrogen serves as an excellent electron donor for many microbial metabolisms, leading to its consumption and contamination. Recent studies have shown that the hydrogen consumption rate can be accelerated by adding solid particles, such as pure quartz grains, into the bulk solution, indicating that solid phases can enhance microbial metabolisms. This raises concerns about the reliability of microbial activity data derived from pure incubation experiments, which may not accurately reflect natural conditions, where hydrogen and microorganisms coexist in rock pore spaces. Rock mineral grains can provide physical attachment sites for microbes, while iron minerals (e.g., hematite) can act as conduits for microbial metabolism, potentially increasing reactivity. Additionally, some minerals may supply essential elements to microbes through dissolution. Therefore, it is crucial to deepen our understanding of bio-geochemical reactions in porous rocks.

Microfluidic experiments offer significant potential for investigating microbial dynamics in porous media. However, microfluidic devices are typically constructed from artificial materials such as PDMS, glass, and silicon, which only replicate pore geometry and fail to capture the chemical and physical properties of natural minerals. We present an approach using real-rock micromodels that combine microfluidic fabrication and thin section techniques using natural sandstones. This method includes rock chemistry and grain surface morphology (e.g., roughness and clay/hematite coatings), features often absent in conventional microfluidics. Additionally, it enables flow-through and incubation experiments with real-time pore-scale imaging. Using these micromodels, we investigated the interactions between methanogenic archaea and rock minerals, focusing on microbial growth, spatial distribution with respect to different minerals, and the impact of biofilm formation on rock permeability and porosity. Preliminary results revealed correlations between gas consumption rates and microbial distribution in Triassic Buntsandstein sandstones.

Within the recently funded Horizon Europe HyDRA project (Diagnostic Tools and Risk Protocols to Accelerate Underground Hydrogen Storage), we aim to advance our understanding of microbial activity in storage sites across Europe. This includes extending the real-rock micromodel approach to incorporate natural microbial cultures from downhole solutions and realistic reservoir materials to study microbial responses when hydrogen is introduced into initially hydrogen-free environments. Key investigations will include changes in wettability, biofilm formation, and their effects on flow properties in natural rocks. Flow-through experiments with microbial communities, including archaea, acetogens, methanogens, and/or Fe^{3+} -reducing bacteria from porous reservoirs, will elucidate the roles of rock minerals and grain surfaces in microbial activity and distribution. Accurate prediction of bio-geochemical reactions and their impact on rock properties will help better assess the risks associated with underground porous storage and develop mitigation strategies.

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MS22 / 60

Additive Manufacturing of Triply Periodic Minimal Surface Structures as Electrodes for Redox Flow Batteries

Author: Maxime van der Heijden¹

Co-authors: Mojtaba Barzegari²; Antoni Forner-Cuenca²

¹ *University of Waterloo*

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Porous electrodes are performance- and cost-defining components of redox flow batteries (RFBs) as they provide the available surface area for electrochemical reactions, the porous structure for electrolyte transport, and facilitate mass, charge, and heat transport [1]. Therefore, enhancing the electrode performance is a promising strategy to increase power density and reduce system costs. Conventional carbon-fiber-based porous electrodes are repurposed from fuel cell gas diffusion electrodes and have not been tailored to sustain the requirements of liquid-phase electrochemistry. Consequently, new manufacturing techniques offering high control over the electrode microstructure and resulting properties need to be developed [2]. Additive manufacturing techniques are uniquely suited to design controlled architectures, which can, in turn, help understand geometry-performance relationships, as well as manufacture high-performance electrodes providing enhanced electrochemical performance and reduced hydraulic resistance [3,4].

I will present our latest progress on the additive manufacturing of advanced electrode geometries for RFBs, illustrating the versatility of this manufacturing approach to fabricate electrode microstructures for electrochemical applications. In this presentation, I will discuss our work on utilizing triply periodic minimal surface (TPMS) structures as RFB electrodes. TPMS structures are found in natural systems such as butterfly wings, leaves, and sea urchin skeletons and have periodic surface structures with large surface areas, which are presumed beneficial for RFB electrodes. In our previous work [4], we found that the electrode pillar shape influences mass transfer rates, motivating the investigation of various TPMS forms, including gyroid, diamond, and IWP. In this work, the TPMS

electrodes were fabricated by additive manufacturing using a commercial desktop digital light processing printer followed by carbonization. We assessed their potential in organic redox flow cells and found that TPMS electrodes feature higher internal surface area and enhanced mass transport compared to cubic periodic structures, boosting the reactor performance. Especially the diamond TPMS outperforms the regular cubic structure, featuring the lowest overpotential and highest current density and mass transfer coefficient. Our work shows the potential of additive manufacturing to fabricate customized porous electrodes that enable multiscale structures with increased electrochemical performance and low hydraulic resistance.

Acknowledgments

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MS06-A / 62

4D X-ray micro-velocimetry during imbibition: snap-off, ganglia remobilization and interfacial drag

Author: Sharon Ellman¹

Co-authors: Robert van der Merwe¹; Sojwal Manoorkar¹; Stefanie Van Offenwert²; Wannes Goethals¹; Christian Schlepütz³; Laurenz Schröer; Tom Bultreys¹

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The simultaneous flow of multiple fluids through a porous medium is important to several earth science applications, such as underground gas storage and groundwater remediation. The intricate interplay between capillary, viscous and gravitational forces inside heterogeneous pore geometries gives rise to non-linear and complex flow dynamics. Even though it is known that imbibition comprises capillary fluctuations which are nonlocal in nature, the temporal and spatial structure of these remain unclear. This is because it was until recently impossible to directly measure unsteady 3D fluid velocity fields in (opaque) porous media.

Recent breakthroughs in 3D X-ray particle tracking velocimetry (Tom Bultreys et al., 2022, 2024) have made it possible to directly measure pore-scale flow dynamics. Here, we use this methodology to investigate imbibition for the first time. We investigate the impact of viscosity ratio at low capillary numbers on unsteady velocity fields during imbibition. To do this, sub-second micro-CT images are acquired at the TOMCAT beamline at the Swiss Light Source while withdrawing the nonwetting fluid from the pore space at a constant, slow flow rate. The nonwetting fluid contains silver-coated hollow glass tracers which are tracked to measure the velocity fields. This enables us to probe the underlying flow dynamics during snap-offs, investigate the effects of interfacial drag on the nonwetting fluid and study ganglia remobilization dynamics. We find that during imbibition displacements, acceleration occurs along tortuous pathways, spanning almost the entire connected oil cluster. Sections of these pathways are then reactivated when the next displacement occurs. When the viscosity ratio is near or less than one, frictional drag along the interface results in recirculation within the nonwetting fluid, similar to what has been seen in micromodel experiments (Roman et al., 2019; Zarikos et al., 2018).

These results are the first pore-scale velocimetry measurements of imbibition in 3D opaque porous materials. These findings inform on the viscous-capillary force balance during imbibition. This will aid in better constraining the time and length scales of energy fluctuations during imbibition, which bears importance to recent theories of energy-dynamics based upscaling (McClure et al., 2021, 2022).

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Poster / 63

Structure Tensor-Based Identification of Laminated Rocks in μ -CT Digital Rock Images

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The identification of lamination patterns in rock samples is important for understanding petrophysical properties behavior in heterogeneous rocks as laminated structures can influence fluid flow patterns, affecting both routine core analysis (RCAL) and special core analysis (SCAL) measurements [1, 2]. Usually, the identification of these structures rely on subjective human interpretation, which can lead to inconsistencies and inefficiencies in large-scale analyses.

Meanwhile, Digital Rock imaging has emerged as a promising approach for automating predictions of petrophysical properties and leveraging rock physics knowledge [3]. However, one aspect often overlooked in Digital Rock analysis is the automation of rock structure characterization, particularly the identification of laminated rock samples. Several aspects can complicate the development of automated methods for identifying these structures from rock images, including varying levels of image noise, diverse lamination types with distinct roughness, frequencies, discontinuities, and orientations characteristics, as well as distinct types of rock heterogeneities and lithologies that could further difficult this process.

In this work, we propose a method for identifying laminated samples from μ -CT images of rock plugs using the structure tensor method. The structure tensor is a mathematical tool that can be used to determine local orientations within images [4, 5]. In our approach, we use these local orientations calculated from the images to compare the distribution of these orientations with a uniform distribution using the Wasserstein distance. Our underlying assumption here is that we expect laminated samples to show a more peaked distribution, indicating a predominant orientation in the image, while non-laminated samples would show a more random distribution that would be closer to a uniform distribution. To determine if a sample is laminated, we adjusted a threshold over the calculated Wasserstein distances based on lamination annotations from three human evaluators. For the lamination orientation, we use the mode of the orientations histogram. Furthermore, we classify each sample into vertical, horizontal, and inclined laminations by comparing the calculated orientation with pre-defined ranges of orientation for each of this categories. A visual representation of our methodology can be seen in the Figure 1.

The proposed methodology is able to distinguish laminated patterns in rock samples and determine their orientation, a crucial aspect for interpreting the impact of these structures on petrophysical properties. Our method has been validated against annotations from three human evaluators across more than 4000 rock μ -CT images, indicating its effectiveness across diverse rock types and lithologies, primarily from carbonate fields in the Brazilian pre-salt formations.

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MS15 / 64

Computer vision benchmark for multi-resolution micro-CT images of carbonate rocks from the Brazilian pre-salt

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A key task in the oil industry is the accurate characterization of pre-salt carbonate reservoir rocks, which display complex heterogeneity at multiple scales. These rocks’ intricate geological structure, shaped by a range of diagenetic processes—such as cementation, dissolution, and fracturing—significantly influences their petrophysical properties [1]. These characteristics demand for cutting-edge characterization methods.

Micro-computed tomography (micro-CT) is a non-destructive technique that creates three-dimensional volumes of objects. In the oil sector, micro-CT of rock samples is often used to evaluate properties like permeability, porosity and fluid connectivity. Furthermore, artificial intelligence (AI), particularly deep learning, has emerged as the state-of-the-art solution for computer vision tasks. Those models have been successfully applied to tasks including segmentation and classification, aiding specialists during the reservoir characterization [2, 3, 4, 5, 6].

Despite the recent progress, not many datasets of carbonate pre-salt rocks are publicly available, particularly those offering both high- and low-resolution images. This scarcity makes it harder to benchmark methods, validate models, and perform multi-scale analysis which are critical for understanding the hierarchical structure of carbonate reservoirs. The dataset titled “16 Brazilian Pre-Salt Carbonates: Multi-Resolution Micro-CT Images” [7, 8] is an open dataset of micro-CT images of high and low resolutions paired with their segmentations, as exemplified in Figure 1. Each sample’s porosity and permeability are also available.

The objective of this study is to establish benchmarks for image segmentation and the prediction of petrophysical properties using the recently released pre-salt carbonate dataset. We compare different deep learning architectures and work with either 2D slices or whole 3D volumes. In this work, we also analyse how image resolution affect the accuracy of the predictions. In the end, this benchmark could be used as an initial study of the dataset and verify how different methods and data resolutions affect the results of image-based characterization.

¹ - <https://www.digitalrockportal.org/projects/503>

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MS23 / 66

Validating a Massively Parallel Dusty Gas Model for Field-scale Modeling of Underground Hydrogen Storage

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Geological H₂ storage enables long-term (days to months) energy storage and grid services for both grid and off-grid energy feedstock (e.g., solar and wind). Scalable, cost-effective H₂ storage can dramatically increase the efficiency of carbon-free energy and further promote usage. Economic storage requires minimizing losses by diffusion through the caprock and contamination by methane and hydrogen sulfide. However, designing and planning realistic porous media storage sites (e.g., depleted gas reservoirs) via simulations has significant challenges due to hydrogen’s exceptionally small molecular cross-section, light weight, and low viscosity.

Subsurface transport simulators typically predict the behavior of gas transport using a combination of Darcy’s Law for advection and Fick’s Law for diffusion and dispersion. This ad hoc advection-diffusion model (ADM) is a simple and effective model for dilute solutions, which is typical in aqueous systems, but ADM is inaccurate for multicomponent gases as it assumes a common solvent velocity. To accurately model transport of gases in a non-dilute multicomponent solution requires not only modeling the concentration gradient driving transport, but also accounting for the relative velocity and cross section of all gases in the solution.

While H₂ can migrate upgradient under some circumstances potentially common in a storage environment, H₂ flow in porous media can also be dominated by Klinkenberg slip or Knudsen molecular flow while larger and more massive gases (e.g., methane and CO₂) behave more conventionally. Slip flow results in larger apparent permeabilities for H₂ in the reservoir formation, which is desirable during injection and withdrawal but can lead to unwanted caprock permeation causing losses and contamination.

The dusty gas model is one approach that uses the Maxwell-Stefan approach for multicomponent gas diffusion and extends its applicability to transition and rarefied flow by additionally accounting for collisions with the solid, porous media. This model seamlessly spans multicomponent continuum, transition, and rarefied flow. However, implementation of the dusty gas model is challenging as

there are no tractable explicit solutions for the flux of each gas species for non-dilute multicomponent systems. Here, direct linear solvers are utilized to solve for the flux of each species in a multicomponent system. Under the assumption of creeping flow, these equations are time-independent and are embedded into fully implicit time, finite volume models for mass and energy. This model has been implemented using the finite volume framework of the subsurface flow and transport code PFLOTRAN and massively parallel non-linear solvers of PETSc.

To validate the dusty gas model implementation, three test cases will be presented. The first is comparison is against steady-state experimental data of countercurrent helium and argon transport through low-permeability graphite ($3.1 \times 10^{-18} \text{ m}^2$) [1][2]. The second comparison is against transient diffusion of a ternary mixture of $\text{H}_2\text{-N}_2\text{-CO}_2$ [3], demonstrating it is capable of modeling “reverse” diffusion due to the entrainment. Finally, the scalability to larger systems, such as permeation through caprock in an underground hydrogen storage system, is demonstrated to assess the feasibility of applying this model to geologic systems.

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Poster / 68

From Fracture Roughness to Fault Conductivity: A Probabilistic Framework for Multi-Scale Uncertainty in CO₂ Leakage Risk Assessment

Authors: Sarah Perez¹; Florian Doster¹; Julien Maes¹; Hannah Menke¹; Ahmed H. Elsheikh¹; Andreas Busch¹

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Quantifying uncertainties associated with fault-related leakage is a significant challenge to ensure safe and efficient storage of CO_2 in the subsurface. The complexity of this problem arises from structural uncertainties in fault damage zones across various scales, which remain poorly resolved. These uncertainties range from seismically sub-resolved fractures to fine-scale structural and material features, such as fracture wall roughness, that are typically neglected in large-scale modelling and can lead to significant model misspecifications. To reliably quantify potential CO_2 leakage rates, it is thus crucial to understand how uncertainties on both the data and models propagate across the scales and influence larger-scale predictions of fracture flow and fault conductivity.

This study directly addresses these challenges by proposing a robust uncertainty quantification (UQ) framework for estimating fracture hydraulic conductivity. The approach is grounded on a probabilistic model that employs Bayesian inference, combining data-driven approaches with physics-based correction of the previous model misspecifications. The framework dynamically adjusts to different sources and magnitudes of uncertainty through adaptive, task-specific weighting, enabling to mitigate modelling and data uncertainties, and improve their predictive capabilities.

A critical insight of our work is that traditional reliance on mechanical aperture measurements alone is insufficient for accurately characterizing flow behaviour in rough fractures. Fracture wall roughness introduces geometric effects that significantly alter hydraulic conductivity and lead to overestimations of the permeability either through the empirical Cubic Law or Darcy flow-based upscaling. To address this, we propose an automatic geometrical correction to infer latent hydraulic aperture fields that account for these roughness effects. This correction enhances the robustness of the modelled hydraulic properties while simultaneously quantifying their associated uncertainties.

Our approach produces detailed hydraulic aperture and permeability maps, with their associated uncertainties, which are crucial for robustly characterizing fracture conductivity derived from the mechanical aperture observations. Moreover, these mappings are designed to be upscaled to larger and more complex fracture networks. This multi-scale capability ensures that the influence of smaller-scale uncertainties, such as those stemming from roughness and sub-resolution features, remains integrated into larger-scale models, preserving essential information for risk assessment and decision-making.

Overall, this work highlights the importance of addressing uncertainty propagation across scales in fault-related leakage problems. By integrating advanced UQ methodologies, it provides a pathway for improving predictions of CO_2 leakage risks, thereby supporting safer and more efficient carbon storage solutions.

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Poster / 69

Pore-scale insights on hysteretic behaviour during cyclic injection in porous media

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Effective underground hydrogen storage in porous rocks requires handling cycles of storage and withdrawal while minimising residual gas saturation, which represents an irrecoverable loss of stored gas and significantly impacts economic feasibility. We will present our recent results on numerical and experimental developments focusing on micromodel systems to investigate these phenomena. The numerical tool is designed to track the pore-scale invasion dynamics under cyclic conditions. Our experimental setup aims to investigate the effects of solid deformation and pore

structure on trapping behaviours under quasi-2D conditions using microcell models. We emphasize the observed cyclic and hysteretic behaviour of residual saturation, highlighting the notable differences between the continuous and cyclic injection scenarios. Furthermore, the effects of pore topological features and solid deformation on hydrogen retention will be explored, showing the importance of pore-scale features and their interplay with the wettability and injection scenarios. Finally, the need to develop a constitutive model designed to capture these cyclic features will be discussed for providing essential tools for optimising underground gas storage options.

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MS26 / 70

Temporal Dynamics of Reactive CO₂ Flow in Carbonate Rocks: Insights from 4D Synchrotron Imaging

Author: Azibayam Amabogha¹

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This study investigates the dynamics of reactive CO₂ transport in carbonate rock, emphasizing the effects of carbonic acid-induced formation damage. We provide real-time visualizations of these processes using 4D high-resolution synchrotron imaging at the I13 beamline at Diamond Light Source. The research captures and quantifies the temporal effects of reactive CO₂ transport at the pore scale in carbonate rock. During the experiment, CO₂-saturated brine was injected into the sample for 5 hours, with 12 images acquired to monitor different stages of chemical dissolution. The fluid was injected at 0.04 ml/min under 8 MPa pressure and 50°C conditions, simulating rapid flow in the near-wellbore region. Image analysis reveals a channelized dissolution pattern accompanied by a gradual increase in porosity due to changes in the pore structure. Pore network models derived from segmented images were used for drainage and imbibition simulations, which indicated a reduction in capillary entry pressure as pore connectivity increased post-dissolution. Additionally, trapping efficiency was quantified, revealing a slight decline with dissolution as pores widened and became more interconnected.

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MS01 / 71

Real time micro-CT imaging of gas-gas mixing in the presence of brine

Author: Samuel Jackson¹

Co-authors: Gulce Kalyoncu ; Sharon Ellman ²; Tanguy Le Borgne ³; Tom Bultreys ⁴

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Hydrogen storage in depleted gas fields is being explored to store large-scale excess renewable energy and alleviate fluctuations in energy demand. The mixing of injected hydrogen with residual natural gas, and the purity of the produced gas stream is controlled by pore-scale mechanisms such as gas-gas mixing through diffusion, dispersion and advection, and large-scale features such as the caprock structure, permeability and brine distribution. The coupled mixing process in partially saturated media is poorly understood.

To this end, we probe the pore-scale mixing of hydrogen in depleted gas fields through time-resolved, two-component, two-phase X-Ray micro-CT experiments in a sandstone rock sample. To resolve the pore-scale gas concentration fields, we use krypton and nitrogen as analogues for natural gas and hydrogen, respectively. The analogue fluids have comparable flow dynamics to their reservoir counterparts (Mobility ratio, Capillary, Bond and Peclet number), but crucially at high pressure, krypton is highly attenuating to X-rays compared to nitrogen. Using the EMCT scanner at Ghent University, we could resolve the relative gas concentrations with a 12-micron spatial resolution and 40-second temporal resolution in a 6 mm diameter sample.

We performed core flood experiments at elevated pressure and temperature, tracking the gas-gas mixing and brine displacement. To mimic the field-scale process, we setup a residual trapped krypton sample (i.e. a depleted gas field), then injected nitrogen (i.e. hydrogen storage) followed by a period of back-production (i.e. hydrogen production), whilst dynamically imaging the core. We performed three experiments, with varying saturation and connectivity of the initial krypton distribution to mimic different field conditions. For the first-time, we were able to visualise and quantitatively analyse the mixing of binary gases in the pore-space, in both connected gas regions, and residually trapped regions. We captured the interplay between advection and diffusion, as well as the simultaneous displacement of brine by both gases. We observed connectivity limited mixing, whereby the connectivity of the gas phase limited the diffusive mixing of the gases, which could play an important role in the field-scale recovery process. We link the mixing statistics to both single and multiphase measures, elucidating the key controls on multi-component multi-phase mixing.

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MS23 / 75

Can a hydrodynamic model predict the flow evolution of a hydrogen plume in a depleted natural gas reservoir?**Author:** Saeed Sheikhi¹**Co-author:** Morris Flynn¹¹ *U. Alberta***Corresponding Authors:** mrflynn@ualberta.ca, sheikhim@ualberta.ca

Hydrogen storage in depleted natural gas reservoirs is a promising solution for storing excess renewable energy on a timescale longer than can be accommodated by salt cavern storage. However, commercial exploitation of the technology in question, and the associated repurposing of an otherwise “dead asset,” awaits the resolution of key challenges and uncertainties. Chief among these from a fluid mechanics perspective is to resolve the connection between hydrogen leakage and the mixing of hydrogen and cushion gas. COMSOL-validated reduced-order-models examining this question have been developed i.e. by Sheikhi and Flynn (J. Fluid Mech., vol. 984, A33, 2024), however their work relies much more heavily on fluid mechanics than it does on thermodynamics. It is therefore unclear the extent to which Sheikhi & Flynn’s model predictions are accurate when compared with e.g. the numerical output from reservoir-level simulation packages. Addressing this knowledge gap is the key focus of the present study. To this end, we use OpenGoSim and CMG to numerically resolve hydrogen injection directly below an interbed layer of reduced, but still finite, permeability. The resulting comparison demonstrates that the theoretical model predicts, with generally good accuracy, the overall shape of the injectate plume plus the amount of hydrogen that dispersively mixes into the surrounding cushion gas. However, reduced-order-model fidelity suffers when the injection time is long, the draining layer is thin and the interbed layer admits a relatively large drainage. This observation highlights areas of future improvement for the reduced-order-model, which can otherwise be applied, with great computational efficiency, in screening candidate depleted reservoirs for their hydrogen storage potential.

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Sheikhi, S. and M.R. Flynn, 2024: Can a hydrodynamic model predict the flow evolution of a hydrogen plume in a depleted natural gas reservoir? *Intl. J. Hydrogen Energy*, 81, 795–804.

MS21 / 76

Inertial effects on tortuosity

Authors: Maciej Matyka¹; Damian Śniezek¹; Sahrish Naqvi¹; Dawid Strzelczyk¹

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We will present our latest observations on tortuosity in pore scale porous media model under high Reynolds numbers (Re) during the transition from the Darcy to the non-Darcy, inertial regime [1]. Unexpectedly, we found that tortuosity does not follow a natural monotonous decrease with increasing flux. We will provide an overview of the method and algorithms employed. Then, we will discuss how we understand the physical mechanisms in the flow causing observed ambiguity. In analyzing our findings, we highlight the significance of inertial effects, the kinetic energy distribution and confinement within the vortices emerging in the flow.

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References:

<https://doi.org/10.1103/PhysRevE.110.045103>

Poster / 77

Cauliflower shapes of bacterial clusters in the off-lattice Eden model

Authors: Maciej Matyka¹; Szymon Kaczmarczyk¹; Damian Śniezek¹; Filip Koza¹

¹ *Faculty of Physics and Astronomy, University of Wrocław*

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We will present our results of an off-lattice Eden model used to simulate the growth of bacterial colonies in the three-dimensional geometry of a Petri dish [1]. In contrast to its two-dimensional counterpart, our model takes a three-dimensional set of possible growth directions and employs

additional constraints on growth, which are limited by access to the nutrient layer. We rigorously tested the basic off-lattice Eden implementation against literature data for a planar cluster. We then extended it to three-dimensional growth. Our model successfully demonstrated the non-trivial dependency of the cluster morphology, non-monotonous dependency of the cluster density, and power law of the thickness of the boundary layer of clusters as a function of the nutrient layer height. Moreover, we revealed the fractal nature of all the clusters by investigating their fractal dimensions. Our density results allowed us to estimate the basic transport properties, namely the permeability and tortuosity of the bacterial colonies.

[1] Szymon Kaczmarczyk, Filip Koza, Damian Śnieżek, and Maciej Matyka, Cauliflower shapes of bacterial clusters in the off-lattice Eden model for bacterial growth in a Petri dish with an agar layer (accepted in Phys. Rev. E)

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<https://arxiv.org/abs/2406.20011>

Poster / 78

Surrogate Modeling of Heat Transfer in Heterogeneous Geothermal Reservoirs Using Finite Volume Informed Graph Neural Network

Author: Reza Najafi-Silab¹

Co-authors: Hannah Menke¹; Florian Doster¹; David Egya¹; Julien Maes¹

¹ *Heriot-Watt University*

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Heterogeneity in underground porous formations stems from the changes in petrophysical properties, such as porosity and permeability, and it can significantly affect the flow patterns and transport phenomena. Accordingly, there has been a long-standing interest in modeling and characterizing heat propagation in heterogeneous geothermal reservoirs to formulate feasible and economic development plans. In this regard, reservoir simulations can get computationally expensive in the case of complex geologic structures. On the other hand, machine learning-assisted surrogate models may be a strong contender for the rapid evaluation of such porous layers based on previously learned fluid and heat behavior. In this work, we utilize the predictive capabilities of deep learning algorithms, learning mesh-based simulation with graph neural networks, to tackle this problem and predict temperature distribution when heterogeneity is intensified or reduced in geothermal systems. Various simulations were carried out for different porosity and permeability distributions using MATLAB reservoir simulation toolbox (MRST) and were employed to train the graph-based predictor. The developed surrogate model has the potential to predict temperature profiles through unseen heterogeneity distributions. This approach would significantly reduce the computational load of simulations and provide a swift method to perform sensitivity analysis and uncertainty assessment while maintaining the complexity of the heterogeneous rock matrix.

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MS07 / 79

A relaxation method for nonlinear convection-diffusion processes with discontinuous terms**Authors:** Arthur Espírito Santo¹; Eduardo Abreu²; John Pérez³; Wanderson Lambert⁴¹ *Universidade Federal do Rio Grande do Sul*² *University of Campinas, Sao Paulo, Brazil*³ *Instituto Tecnológico Metropolitano –ITM, Medellín, Colombia*⁴ *UNIFAL***Corresponding Authors:** arthurmes@ufrgs.br, eabreu@ime.unicamp.br, jhonperez@itm.edu.co, wanderson.lambert@gmail.com

We propose a mathematical relaxation method for nonlinear partial differential equations of convection-diffusion type discontinuous terms and computational applications [1,2]. We reformulate the underlying convection-diffusion problem as a system of hyperbolic equations coupled with relaxation terms. In contrast to existing literature on relaxation modeling (see, e.g., [3,4] and the references cited therein), where the solution of the reformulated problem converges to certain types of hyperbolic conservation laws as the limit of equations involving regularizing higher order terms in the possible mixed diffusive/dispersive limit, our formalism treats the augmented problem as a system of coupled hyperbolic equations with relaxation acting on both the convective flux and the source term [1,2,5]. We have shown the new system of equations satisfies Liu's sub-characteristic condition. Further, we present several one-dimensional numerical experiments, including nonlinear convection-diffusion problems with discontinuous coefficients motivated by discontinuous capillary pressure for two-phase flows in porous media, aiming to illustrate the feasibility of the approach.

[1] E. Abreu, W. Lambert, A. M. Espírito Santo and John Perez. A relaxation approach to modeling properties of hyperbolic-parabolic type models, *Communications in Nonlinear Science and Numerical Simulation*, Volume 133 (2024). LINK: <https://doi.org/10.1016/j.cnsns.2024.107967>.

[2] E. Abreu, P. Ferraz, W. Lambert. A study of non-equilibrium wave groups in two-phase flow in high-contrast porous media with relative permeability hysteresis, *Communications in Nonlinear Science and Numerical Simulation*, (2023). LINK: <https://doi.org/10.1016/j.cnsns.2023.107552>.

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[4] S. Jin, L. Pareschi and G. Toscani, Diffusive relaxation schemes for multiscale discrete-velocity kinetic equations. *SIAM J Numer Anal* 1998;35(6):2405-39. LINK: <https://doi.org/10.1137/S0036142997315962>

[5] E. Abreu, A. Bustos, P. Ferraz and W. Lambert (2019), A Relaxation Projection Analytical-Numerical Approach in Hysteretic Two-Phase Flows in Porous Media. *Journal of Scientific Computing*, v.79, p.1936. LINK: <https://link.springer.com/article/10.1007%2Fs10915-019-00923-4>

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

E. Abreu, Associate Professor, Department of Applied Mathematics – <http://www.ime.unicamp.br/~eabreu/>
| University of Campinas - UNICAMP, Brazil – <https://www.unicamp.br/en>

MS25 / 80

Strategies for overcoming the challenge of gigaton-per-year basalt carbonation

Author: Benjamin Tutolo^{None}

Co-authors: Adedapo Awolayo¹; Bohyun Hwang²; Jianwei Tian¹; Madeline Bartels²; Matthew Eisaman³; Qin Zhang⁴

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² *University of Calgary*

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Basalt carbonation has gained traction as a large-capacity technique to manage atmospheric carbon dioxide (CO₂) concentrations and potentially avoid the most dramatic impacts of climate change. Yet, while several successful injection operations have demonstrated the efficacy of this technique at the scale of thousands of tons of CO₂ injected per year, achieving the necessary impact on atmospheric CO₂ concentrations will require expansion to the gigaton-per-year scale. However, implementing basalt carbonation at this scale will face important geochemical and hydrogeological challenges. At the gigaton-per-year scale, maximizing per-well CO₂ injection rates will likely involve injecting CO₂ in a supercritical, rather than dissolved, state, which will, in turn, lead to less efficient basalt carbonation (Tutolo et al., 2021). To combat this challenge, we are exploring alternative injection strategies, including Water-Alternating-Gas injection (Awolayo et al., 2025), which will enhance in-situ CO₂ dissolution, as well as an acid pretreatment step that will enhance cation extraction from the basalt prior to, or alongside, CO₂ injection (Zhang et al., 2024). Moreover, sub-optimal –in terms of lower reactivity, and non-ideal permeability and porosity –basaltic aquifers will need to be exploited to help us achieve gigaton-scale basalt carbonation. To explore methods for combatting these challenges, we are examining their effects using a combined experimental and reactive transport modeling approach. Our initial laboratory experiments indicate decreased reactivity of altered, lower-reactivity basalts relative to pristine and/or glassy basaltic counterparts. However, our simulations incorporating hydrogeologic heterogeneity indicate that heterogeneous aquifer permeability and porosity tend to increase rates of mineralization relative to simulations incorporating idealized isotropic, homogenous aquifers. Finally, we are exploring the possibility that the acid pretreatment step utilized to enhance cation release may also enhance permeability and pore connectivity in tight aquifers. Ultimately, our results indicate that achieving the substantial promise of basalt carbonation as a climate change solution will require innovative solutions to a wide variety of challenges not generally investigated in existing laboratory and field-scale studies.

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MS15 / 82

Scaled-cPIKANs for Porous Media Flows: Chebyshev-based Physics-informed Kolmogorov-Arnold Networks**Author:** Farinaz Mostajeran¹**Co-authors:** Nicholas T Baker¹; Salah A Faroughi¹¹ *University of Utah***Corresponding Authors:** nicholas.t.baker@utah.edu, salah.faroughi@utah.edu, u6060918@utah.edu

Fluid flow and transport phenomena in heterogeneous porous media have diverse applications in science and engineering fields. These processes are dominated by steep gradients, non-linear interactions, and multi-scale phenomena, rendering the governing equations, aka PDEs, exceedingly complex and computationally demanding to solve. Although decades of research have led to several breakthroughs in numerical techniques, there remains a substantial demand for faster and more scalable methods to solve these complex PDEs. This field of research has intensified significantly with the advent of PDE-solvers driven by neural networks. In particular, advances like Physics-Informed Neural Networks (PINNs) have transformed this domain by introducing mesh-free frameworks that inherently embed multi-scale physical laws into their architecture. This capability is very significant for multi-scale transport phenomena with complicated boundary conditions, as there is no need to use conventional grids, hence paving a pathway to scalability with efficient solutions.

Building on this foundation, this work introduces Scaled-cPIKAN, a novel physics-informed neural network architecture that combines Chebyshev polynomial-based representations with domain scaling techniques. Scaled-cPIKAN integrates the mathematical flexibility of Kolmogorov–Arnold Networks (KANs) with the physics-informed concepts of PINNs, and utilizes Chebyshev polynomials as basis functions to accurately capture high-frequency fluctuations and fine-scale flow features. By scaling the governing PDEs and normalizing the input data, Scaled-cPIKAN enhances the network's ability to model complex dynamics in extended spatial domains, reducing computational overhead and improving accuracy. Key features include efficient handling of sharp gradients, oscillatory behaviors, and the ability to solve problems in large domains without requiring dense collocation points and/or deep architectural frameworks (e.g., layers and nodes). To highlight these features, we apply the proposed Scaled-cPIKANs model to solve the advection-diffusion and reaction-diffusion problems. Our results show that, unlike vanilla PINNs and KANs that suffer from oscillations and degradation in accuracy over large domains, the Scaled-cPIKAN approach provides robust convergence rates with high accuracy without excessive computation and data burdens. These improvements stem from the synergistic effect of domain scaling and adaptive Chebyshev polynomial representation, which improve the expressiveness and convergence properties of the network. Thus, Scaled-cPIKAN proves to be an effective model for solving real-world multi-scale transport phenomena in porous media that require significant computational efficiency and accuracy.

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MS24 / 83

Machine-Learned Force Field Development for Molecular Simulation of CO₂ Adsorption/Desorption in UiO-66 Metal-Organic Frameworks

Authors: Bassam Rabihavi¹; Fateme Rezaei^{None}; Mehdi Vaez Allaei^{None}; Muhammad Sahimi^{None}; Shayan Jalalmanesh¹

¹ *Ph.D. Student*

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Metal-organic frameworks (MOFs) have emerged as highly promising materials for CO₂ capture, due to their tunable porosity, high surface area, and structural versatility. We report on the development of a suitable force field for a widely studied zirconium-based MOF, UiO-66, to explore its potential for direct capture of CO₂. An accurate force field for the MOF is developed using machine learning interatomic potentials (MLIPs). Specifically, we use the Moment Tensor Potentials (MTPs), implemented through the MLIP package. An active learning approach is employed to iteratively refine the force field, ensuring robust and efficient predictions, while minimizing computational cost. The newly developed machine-learned force field enables molecular dynamics simulations of CO₂ adsorption in UiO-66, providing insights into the adsorption capacity, structural stability, and host-guest interactions. The methodology not only captures the adsorption behavior with near DFT-level accuracy, but also highlights the importance of force field reliability in adsorption simulations. Future work will extend this framework to include adsorption selectivity studies and explore the impact of structural modifications on CO₂ uptake.

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Poster / 85

A new phase diagram for fluid invasion patterns as a function of pore-scale heterogeneity, surface roughness, and wettability

Author: Helmut Geistlinger¹

Co-authors: Bilal Zulfiqar²; Mohd Amro³

¹ UFZ

² Helmholtz-Zentrum für Umwelt Forschung- UFZ

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Understanding how different flow patterns emerge at various macro- and pore scale heterogeneity, pore wettability and surface roughness is remains a long standing scientific challenge. Such understanding allows to predict the amount of trapped fluid left behind, of crucial importance to applications ranging from microfluidics and fuel cells to subsurface storage of carbon and hydrogen. We examine the interplay of wettability and pore-scale heterogeneity including both pore angularity and roughness, by a combination of micro-CT imaging of 3D grain packs with direct visualization of 2D micromodels. The micromodels are designed to retain the key morphological and topological properties derived from the micro-CT images. Different manufacturing techniques allow us to control pore surface roughness. We study the competition between flow through the pore centers and flow along rough pore walls and corners in media of increasing complexity in the capillary flow regime. The resulting flow patterns and their trapping efficiency are in excellent agreement with previous μ -CT results. We observe different phase transitions between the following flow regimes (phases): (i) Frontal/ compact advance, (ii) wetting and drainage Invasion percolation, and (iii) Ordinary percolation. We present a heterogeneity-wettability-roughness phase diagram that predicts these regimes shown in Fig. 1 (Geistlinger et al., 2024).

-> include here Figure 1

Figure 1. A) The phase diagram shows the transition in flow regimes from A) frontal advance to B) drainage invasion percolation with increasing contact angle and for uniform porous media (2D glass beads). For porous media with higher heterogeneity/disorder and smooth surface ($y = 0$; Delaunay pore structure, 2D sand) a second transition to wetting invasion percolation is observed. The transitions in displacement regimes are quantified by the finger width, W . B) Phase diagram for porous media with rough surfaces ($y > 0$).

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Geistlinger, H., Golmohammadi, S., Zulfiqar, B., Kuechler, M., Reuter, D., Schlueter, S., . . . Amro, M. (2024). A new phase diagram for fluid invasion patterns as a function of pore-scale heterogeneity, surface roughness, and wettability. *Water Resources Research*, 60 (6), e2023WR036036.

The mechanism of CO₂ huff and puff and the distribution characteristics of micro-nano pore fluid in shale reservoirs

Authors: Jiajing Chang¹; Zhaojie Song²

¹ China University of Petroleum (Beijing) & Sinopec Petroleum Exploration and Production Research Institute

² China University of Petroleum (Beijing)

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CO₂ huff and puff plays a key role in the development of shale oil. At present, there are few studies on the production law of micro-pore crude oil in the process of CO₂ huff and puff from the perspective of shale pore structure, and quantitative analysis of the lower limit of pore size in CO₂ huff and puff and CO₂ action distance.

Firstly, the pore size distribution of rock samples was determined by high pressure mercury injection and nitrogen adsorption experiments. The fracture development degree of rock samples was scanned by CT, and then the NMR experiments of CO₂ huff and puff and water injection + CO₂ huff and puff were carried out. The effects of huff and puff cycles, fracture development degree and injection type on the seepage law of shale oil were studied from the microscopic scale.

The results of one-dimensional T₂ spectrum scanning showed that the oil production of matrix/matrix-fractured shale in the process of CO₂ huff and puff mainly depended on the first two rounds. The results of CT + MRI imaging scanning showed that the pore connectivity of matrix shale was good, and CO₂ mainly used crude oil in the surrounding area of core in the initial stage. Matrix-fractured shale fractures accounted for a relatively high proportion (11.55 %). In the initial stage, CO₂ mainly used crude oil in fractures and the surrounding areas of fractures. The results of one-dimensional frequency coding scanning showed that the utilization degree of crude oil at the inlet end was the best, and the farther away from the inlet, the utilization degree of crude oil was worse. Water injection + CO₂ composite huff and puff could significantly improve the degree of crude oil recovery, and the effect was mainly reflected in the outlet end.

The research results can better reveal the mechanism of enhanced oil recovery by CO₂ huff and puff and clarify the influence of different factors on enhanced oil recovery by CO₂ huff and puff, and optimize a reasonable injection method, which provides theoretical support for injection development and effect evaluation of shale reservoirs.

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PETROPHYSICAL CHARACTERIZATION OF INDIANA LIMESTONE USING MEDICAL DUAL-ENERGY COMPUTED TOMOGRAPHY TECHNIQUE: INSIGHTS INTO POROSITY, BULK DENSITY, AND EFFECTIVE ATOMIC NUMBER

Author: Walter Leonardo Flores Antelo¹

Co-authors: Janeth A. Vidal Vargas¹; Jose E. Chiarelli¹; Rosangela B. Z. L. Moreno¹

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Computed Tomography (CT) images enable non-destructive 3D reconstruction of pore structures and mapping of rock properties. Typically, such images are obtained from high-resolution acquisitions using micro-CT scans (10–6 m) or synchrotron beamlines (10–9 m). The quality of these images is further enhanced through preprocessing steps such as filtering, cropping, masking, and contrast enhancement. However, high-resolution acquisitions are constrained by their time-consuming, high costs, and limitations on sample size, which restrict the representative elementary volume (REV) and its ability to accurately represent the sample's heterogeneity. To address these challenges, this study aims to characterize petrophysical properties of rock samples, including porosity (ϕ), bulk density (ρ_b), and effective atomic number (Z_{eff}), using medical-CT resolution (10–4 m) with the dual-energy CT technique (DECT). We analyzed six Indiana limestone samples, each with a diameter of 3.81 cm and an approximate length of 4.88 cm. The samples have a porosity range of 17.5% to 19.1%. Low-resolution images (100 μ m) were acquired using medical-CT scans with high-energy (130 kVp) and low-energy (80 kVp) acquisition and reconstruction protocols. These paired images served as inputs for DECT. As a result, we generated 2D/3D maps of key properties (ϕ , ρ_b , Z_{eff}), profiles along the sample length, and averaged values. These quantitative and qualitative results allow for the identification and visualization of sample property heterogeneity, a defining characteristic of this type of carbonate rock. Additionally, the single-energy CT technique (SECT) was applied to each sample, using enhanced images obtained by subtracting the saturated sample images from the dry sample images. This approach improved the contrast of the effective porosity. DECT and SECT results for each sample were obtained using in-house Python code and image preprocessing performed with Avizo 3D. This study demonstrates that the medical-CT for petrophysical characterization offers a faster, cost-effective solution that allows for the analysis of considerably larger samples, overcoming the limitations of traditional high-resolution imaging techniques. The methodology provided reliable and accurate estimation for bulk density, porosity and effective atomic number, highlighting its potential for characterizing key petrophysical properties.

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Water & Porous Media Focused Abstracts:**References:**<https://doi.org/10.2118/90520-MS>

MS24 / 88

Molecular Modeling of the Structure and Dynamics of Nanoconfined Fluids

Author: Jeffery Greathouse¹¹ Sandia National Laboratories**Corresponding Author:** jagreat@sandia.gov

Understanding the structure and dynamics of fluids at nanoconfined interfaces is essential for continued progress in subsurface energy and environmental applications, and industrial applications such as catalysis, adsorption, and separations. Nanoscale structural, spectroscopic, and transport properties are readily obtained from molecular dynamics (MD) simulation, allowing the effects of

fluid chemistry, pore surfaces, and pore size to be explored. Results will be presented for recent MD studies of nanopores comprised of amorphous silica and other materials, as well as a new force field for simulating bulk silica phases and silica-water interfaces. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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Dynamic evolution laws and mechanisms of high-temperature steam seep-age and coal thermal strain during injecting steam into coal

Author: zhiqiang Li¹

Co-author: lin li ¹

¹ *Henan polytechnic University*

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Thermal excitation of coal seams by high-temperature steam is a highly promising technology to increase gas production. Among them, steam permeability is a key parameter characterizing the injection capability of thermal fluids. However, the seepage law of steam in coal and its evolution mechanism are still unknown. In order to solve the above problems, experiments were carried out to determine the permeability and thermal strain of high-temperature steam in coal, and the evolution law of the permeability of high-temperature steam and thermal strains of coal was obtained. The experiments found that during the process of high-temperature steam injection into coal, with the extension of the injection heat time, the liquid-measured permeability shows an intermittent oscillation law. With the increase of steam temperature, the peak values of the oscillation decrease, the periods are shortened, and the oscillation is more intense. During the heat injection process, the radial and volumetric strains of the coal show 2~3 expansion stages. When the steam temperatures are low, the axial strains are compressive, and when the temperatures are high, the axial strains turn to expansion. The theories of Kelvin capillary condensation, plug flow and thermal stress were used to investigate the mechanisms of condensation phase change, oscillatory seepage of steam and thermal strains change of coal, respectively. The study shows that the equilibrium pressure of steam in the micro-pores of the coal is less than the saturated vapor pressure in the large space, and the smaller the pore diameter, the lower the pressure required for steam condensation, and the easier steam condense. The gas-liquid plug flow induced by steam in the coal is the main mechanism causing intermittent oscillation of permeability. In addition, the high-temperature steam has superimposed inward and outward expansion influence effects on the permeability of the coal, leading to a decrease in the permeability of large pores and an increase in that of small pores in the matrix. During the steam injection process, the rapid expansion strains in the early stage are mainly controlled by the pore pressure, and the slow expansion strain in the middle and late stages by the thermal strain. The results provide factual basis and theoretical reference for the practice and numerical simulation of steam thermal recovery gas.

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References:

90

Probing Primer Penetration Dynamics in Coated Paper Using Ultra-Fast NMR Imaging

Author: Isik Arel¹

Co-authors: Henk Huinink¹; Bart Erich²; Olaf Adan²; Luc van Keulen³; Nicolae Tomozeiu⁴

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The interaction of liquids with thin porous media is fundamental across various applications, such as printing [1], coating [2], and paper-based microfluidics [3], where controlled fluid transport is essential for performance optimization. In industrial printing processes, primer liquids are specifically formulated to prepare porous substrates by modifying their surface properties and ensuring controlled absorption of subsequent colorful ink layers. This preparation is essential to achieving uniform ink distribution, vivid color reproduction, and improved print quality.

This study focuses on understanding the penetration dynamics of primer liquids into coated paper—a fibrous, multi-scale porous substrate—using ultra-fast Nuclear Magnetic Resonance (UFI-NMR) imaging. The UFI-NMR system provides real-time, non-invasive measurements by tracking the spatially resolved signal intensity of the liquid phase within the substrate, offering high spatial resolution and a temporal resolution of 10 μ s, captured every 10 ms, to monitor rapid capillary-driven penetration processes [4]. This enables precise quantification of key transport parameters, including penetration depth, propagation speed, liquid distribution, and substrate swelling.

The primer liquid used in this study is formulated with metal salts as active agents and surfactants, whose concentrations are systematically varied to examine their influence on fluid transport. This systematic investigation reveals how the combined action of metal ions and surfactants modulates penetration by altering fluid viscosity, surface interactions, and pore-scale transport mechanisms.

Overall, this study demonstrates how UFI-NMR imaging can be employed to investigate capillary-driven absorption dynamics and diffusion behavior in coated paper substrates. The findings contribute to optimizing primer formulations for enhanced inkjet printing quality.

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Water & Porous Media Focused Abstracts:**References:**

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A multi-scale multi-step machine learning method for absolute permeability estimation from porous media low resolution medical-CT images

Author: Eduardo Bueno¹

Co-authors: José Maria Herrera Saravia ¹; Rosangela Zanoni Lopes Moreno ¹; Walter Leonardo Flores Antelo ¹

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Medical CT imaging is a key tool in porous rock characterization. Its importance stems from its ability to provide large fields of view, enabling acquisitions of core samples of several centimeters in diameter and length. Consequently, analysis of more representative volumes of heterogeneous rocks becomes possible, since larger scale features and higher degrees of variability gets captured. That comes, however, with the downside of low resolution acquired images (voxel lengths greater than 100 μm), making it hard to fully resolve the sample pore space, since many pores, specially for carbonate rocks, will lie in the subresolution scale. Image-based permeability estimation methods, such as Lattice Boltzmann Method (LBM), rely on pore-matrix segmentation. However, LBM canonical form can yield incorrect results for samples with unresolved pores. To overcome this limitation, the present work proposes a multi-scale multi-step machine-learning-based methodology to estimate absolute permeabilities based on medical CT images. To accomplish that, dimensionless features derived from Minkowski functionals of 3D and 2D subdomains of high resolution (8 μm voxel length) micro-CT images of carbonate rocks. These features are matched against absolute permeability values estimated through LBM simulations. As a first step, the extracted features, along with the porosity of each subdomain, are subjected to an unsupervised classification model which identifies clusters of subdomains and labels them. Secondly, neural networks are employed in a regression step to find Kozeny-Carman parameters for each of the identified labels. Finally, based on the hypothesis that carbonate rocks display self-similar (or fractal) properties, a porosity and a segmented image of a 30 cm wide and 3.81 cm diameter carbonate core sample acquired through medical CT are subjected to the classification and regression models. With the sample subdomain types identified through the segmented image, the Kozeny-Carman models found by the neural networks are employed to estimate the permeabilities of the subdomains using the porosity image. Employing the proposed methodology, the absolute permeability of the sample was estimated to be 83.8 mD while core-flooding measurements indicate a permeability of 88.2 mD, representing an error of 5%. This result indicates that the fractal hypothesis is valid and that the methodology is reliable.

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Water & Porous Media Focused Abstracts:

References:

Poster / 92

Modeling water imbibition in porous ceramics using Richards equation: Insights into saturation dynamics and role of material properties

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Co-author: Krishna M. Pillai²

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Porous ceramics have diverse applications, including water filtration, heat transfer, catalyst support, and liquid evaporation. They are also essential as water-sealing residential tiles, where understanding water imbibition is crucial for improving tile coating quality. This study focuses on modeling water imbibition using Richards' equation, a complex nonlinear partial differential equation without a closed-form solution in multi-dimensional geometries. Numerical simulations were performed using COMSOL Multiphysics to solve Richards' equation. The research begins by validating the simulation results against neutron microscope imaging (NMI) data, comparing the saturation fronts from simulations and experiments.

Once validated, the simulations were conducted for three scenarios: water droplets on bare ceramic, ceramic with hydrophilic coating, and ceramic infused with hydrophobic particles. Results show that material properties significantly influence the saturation behavior. For bare ceramics, the saturation front is ellipsoidal; for hydrophilic coatings, it resembles a flat surface; and for hydrophobic particle infusion, it becomes irregular. While the saturation levels across all cases increase over time, the saturation front slows down and flattens, becoming less curved with time. This study provides valuable insights into the effects of material properties on water imbibition, enhancing our understanding of processes crucial for improving ceramic coatings in various applications.

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References:

MS17 / 93

Sharp-front models for wicking into porous media under non-isothermal conditions

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Wicking, the spontaneous movement of liquid into a dry porous medium, is a critical phenomenon with wide-ranging industrial applications. Though wicking under isothermal conditions have been studied/modeled for more than a century, wicking under non-isothermal conditions remains relatively unexplored.

In an earlier study, we proposed, using the sharp-front approximation, three different models for wicking height as a function of time for the non-isothermal wicking phenomenon. Three temperature models are: the Liquid Temperature Model, the Average Temperature Model, and the Dynamic Temperature Model. The first two models use the Darcy's law based analytical solution for wicking height as a function of liquid properties including viscosity, surface tension and density and where these properties are varied with an estimation of liquid temperature. The Liquid Temperature Model (with the liquid temperature set at the constant temperature of the incoming liquid) incorporates some temperature effects but tends to underestimate the wicking height due to its simplified assumption. The Average Temperature Model improves accuracy by evaluating properties at the average of the liquid and wick temperatures but still falls short, due to its failure in capturing the dynamic nature of energy redistribution during wicking. The Dynamic Temperature Model calculates liquid temperatures along the wick using a 1-D finite difference-based simulation and dynamically computes fluid properties at these varying temperatures along the wick. This model achieves superior predictions of wicking height and successfully captures temperature transitions observed in experiments.

We will be predicting the wicking height of hexadecane at room temperature in a beaker with a polypropylene wick at elevated temperatures (which is the opposite of the situation considered by us earlier with the liquid set at higher temperatures). Similar conditions are commonly encountered in industrial applications, for example, in heat pipes where wicking materials are at higher temperatures compared to the working fluids. This work will provide novel insights into non-isothermal wicking by demonstrating how temperatures influence liquid transport in porous media. The findings hold significant implications for applications in textiles, heat pipes, and advanced cooling systems, where thermal effects are critical for liquid management.

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MS02 / 94

Microfluidics-based experimental study of the use of yield stress fluids to improve organic pollutant removal from contaminated soils

Authors: Zhansaya Aitkhozha¹; Antonio Rodríguez de Castro²; Amine Ben Abdelwahed³; Henri Bertin³

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Urban and agricultural environments are increasingly contaminated by chlorinated solvents, pesticides, nitrates, heavy metals, etc. Such pollutants, which initially impact surface soils, eventually seep into groundwater. It is therefore essential to remediate degraded soils to ensure water and food sovereignty. This study presents a method for remediating soils contaminated by organic pollutants through the selective blocking of local heterogeneities. This technique is based on the use of yield stress fluids, specifically concentrated biopolymer solutions, which, due to their distinctive rheological properties, preferentially flow through larger pores. Once the yield stress fluid is injected, water predominantly moves through smaller pores, thereby redirecting flow to areas that are less accessible during standard remediation operations.

This study presents laboratory experiments performed at the pore scale who were conducted to validate this method and confirm previous findings from core-flooding experiments [1]. To address and confirm these inquiries, we used transparent microfluidic devices that allow flow visualization. Two borosilicate glass micromodels with microchannels representing the topology of a sandstone were used as model porous media. The pore structure of both microchips was identical; however, one was water-wet while the other was oil-wet. Their absolute permeability was 2.5 Darcy, their porosity was 0.58 and their pore volume was 2.4 μl . The pore size distribution of the microchannels was measured on a 2D image of the micromodel mask. The yield stress fluids were aqueous solutions of xanthan gum biopolymer with three different polymer concentrations C_p : 3000, 5000 and 7000 ppm. To enhance differentiation between liquids during multiphase flow in the micromodel, distinct dyes were applied: violet ink in the water at 10 wt.%, green ink in the polymer solution at 10 wt.%, and oil-red-o powder at 3 wt.% in the mineral oil. Aqueous xanthan gum solutions were used to obstruct the larger pores in the micromodels. Image post-processing of the raw images obtained with the microscope camera after each experimental step was performed using ImageJ open-source software. The effects of polymer concentration and flow conditions underscored the benefits of the proposed method. A significant improvement in pollutant removal was achieved with water flow diversion produced by polymer blocking compared to conventional waterflooding in all cases studied in this work. The proposed method enabled significant improvements in pollutant removal with minimal injected pore volumes of polymer and water. The distribution of phases within the pores, the area of pollutant clusters, and the sizes of the pores occupied by each phase were effectively characterized in the current microfluidic experiments.

[1] Rodriguez de Castro A., Ben Abdelwahed A., Bertin H., Enhancing pollutant removal from contaminated soils using yield stress fluids as selective blocking agents. J. Contaminant hydrology. 255, 104142, February 2023

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References:

MS06-B / 95

Absorption and diffusion process at the CO₂-oil interface considering density fluctuations near the critical CO₂ point

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CO₂ injection into geological formations is considered as technologically advanced and economically feasible approach that combines both CO₂ sequestration and enhanced oil recovery (EOR). The absorption- and diffusion processes at the CO₂-oil interface (under reservoir conditions) plays an integral role in governing key physico-chemical properties such as volume increase, miscibility, density change, diffusion, and interfacial tension and their complex interrelationship.

We proposed a conceptual model that accounts for CO₂ density fluctuations in the critical range (31°C, 7.38 MPa) and explains the time-dependent oil volume increase under specific thermodynamic conditions. Our micro-CT experiments validate the model and demonstrates that the oil volume increase in the non-critical pressure range (< 6 MPa) is a surface effect with limited penetration depth, controlled by the lighter/short-chain alkanes in the oil. The oil swelling increase significantly from 1.8 mm to 14 mm by varying the composition of lighter components (C₁-C₁₀) in the oil from 20 % to 100 %, respectively. An ordered short-chain alkane-CO₂-alkane structure forms at the CO₂-oil interface through CO₂ binding bridges subsequently enhancing oil volume until the equilibrium is achieved. In the critical pressure range (6 - 8 MPa), oil volume increase is caused by the mixing of liquid CO₂ droplets in the oil phase.

Concurrently, we conducted independent pressure decay analysis, evaluated the key kinetic parameters, and studied the CO₂ diffusion processes in the oil phase. Our conceptual model shows an excellent agreement (relative error ≤ 0.5 %) with the pressure-decay experimental results for both the equilibrium- and non-equilibrium model, and a diffusion coefficient in the range of 10⁻⁷ m²/s indicates a fast CO₂ mass transfer process.

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References:

Geistlinger, H., & Zulfiqar, B. (2024). Absorption and diffusion process at the CO₂-decane interface considering density fluctuations near the critical CO₂ point. *Surfaces and Interfaces*, 105520.

96

Aquifer Thermal Energy Storage and Production in Gulf Coast Formations using Numerical Simulations

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Aquifer Thermal Energy Storage (ATES) utilizes the abundance of free geothermal energy in the subsurface to reheat the injected fluid, store it in the aquifer and produce it when demand rises. The higher temperature of produced fluid can be used for different applications ranging from electricity generation, household heating, and animal husbandry. We test this hypothesis in moderate temperature aquifers in the Gulf Coast, USA. Multiple scenarios are simulated in this study over a thirty-year period to assess ATES in aquifers of Texas/Louisiana using the SUTRA program. The results indicate that ATES system power output and efficiency are influenced by the distance between injection and production wells, the flow rate, and the cycle schedules. Increased injection/production rates yield the highest power output, followed by a greater distance between wells. Thermal efficiency is maximized through increased well spacing and extended rest periods between ATES cycles. However, setting the ATES system to idle reduces the overall power output compared to maintaining a continuous ATES operation. The research demonstrates the feasibility of implementing geothermal energy in areas where high temperatures are not readily available for a more widespread clean energy source.

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References:

Bershaw, J., Burns, E., Cladouhos, T. T., Horst, A. E., Van Houten, B., Hulseman, P., Kane, A., Liu, J. H., Perkins, R. B., & Scanlon, D. P. (2020). An integrated feasibility study of reservoir thermal energy storage in Portland, Oregon, USA. 45th Workshop on Geothermal Reservoir Engineering,

MS22 / 97

Design of plate-like black bodies at 1000°C based on black metal coatings: effect of their internal micro-porosity on their effective normal spectral emissivity.

Author: Benoit Rousseau^{None}

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In a global context where the decarbonization of high-temperature industrial processes for material transformation or energy conversion is an important issue, heating technologies based on electric radiants are once again being studied. Academic work shows that the best possible electric radiant is one whose directional spectral emissivity is analogous to that of the Planck black body as shown by the thermal balances involving a radiant source and a receiver to be heated. Commercial radiants are far from having this propensity, due to the choice of refractory materials used: semi-transparent alumino-silicate ceramics, refractory metal alloys with moderate emissivity, carbon ribbons with higher emissivity but having to work in a protective atmosphere, silicon carbide ceramics with high emissivity that become brittle at 900°C due to chemical corrosion. An original, but little-known approach consists of creating a coating of mixed rare-earth oxide with very high emissivity on the

surface of an electric plane radiant (200643 mm, 1000 and 1500 W) made of cordierite-mullite. As long as the microscopic mechanisms responsible for the oxide's intrinsic high emissivity are active, the overall radiative character is pseudo-blackbody-like. The thermal-radiative data available to date on this family of oxides shows that a operating temperature of 1000°C under air can be targeted today. Electrical data suggest that higher working temperatures can be achieved. In this work, we will show how the use of high-temperature X-ray μ -tomography combined with scanning electron microscopy can highlight the crucial role of the micro-porosity of high-temperature spray-pyrolysis Pr_2NiO_4 +d deposits in their high-temperature radiative behavior. Multi-scale modeling combining a macro-scale ray-tracing method, a meso-scale Maxwell-Garnett model and a micro-scale Drude-Lorentz model confirms the key role of this internal micro-porosity. We will discuss the link between the elaboration process put in evidence, the dual-scale texture of the deposits and the thermal radiative properties obtained. The challenges posed by this study will also be discussed, ranging from characterizing the radiative properties of these coatings up to 1500°C, to characterizing micro-porosity using advanced methods (X-ray nano-tomography, USAXS, SANS, FIB-SEM, etc.) up to choosing effective media laws that take into account possible cooperative electromagnetic effects. Considerations for large-scale industrial deployment (900 MW steam cracking furnace, foundry furnace) will also be addressed.

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References:

MS01 / 98

From natural gas storage to hydrogen storage: Microscopic flow dynamics of hydrogen versus methane in fractured reservoir rock

Author: Sojwal Manoorkar¹

Co-authors: Gulce Kalyoncu²; Hamdi Omar²; Soetkin Barbaix¹; Dominique Ceusters³; Maxime Latinis³; Stefanie Van Offenwert¹; Tom Bultreys¹

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Underground hydrogen storage offers a promising solution for addressing seasonal renewable energy fluctuations. While converting natural gas storage facilities to hydrogen storage leverages existing infrastructure, the differences in flow behavior between hydrogen-brine and methane-brine systems, particularly through fractures and sealing caprock, remain poorly understood. This study investigates the pore-scale two-phase flow dynamics of hydrogen, methane, and their mixtures in fractured limestone from the Loenhout natural gas storage facility in Belgium. Controlled primary drainage (gas injection) and imbibition (withdrawal) experiments were conducted at typical reservoir conditions (10 MPa and 65°C) on three different rock samples, revealing the impact of fracture geometry on fluid invasion patterns and recovery efficiency. Our results show that H_2 and CH_4 exhibit similar gas saturations after primary drainage, but H_2 forms larger numbers of smaller ganglia compared to CH_4 due to more discontinuous invasion in rough fractures. The flow through

fracture is influenced by variable aperture and roughness on flow dynamics, gas trapping, and recovery efficiency. Furthermore, steady-state relative permeability experiments on fractured carbonate rock from Loenhout show that the relative permeability for hydrogen is similar to methane but significantly lower than for nitrogen, implying that nitrogen cannot serve as a reliable proxy for hydrogen in typical reservoir conditions. This study emphasizes the need for accurate pore-scale modeling to inform field-scale predictive models for underground hydrogen storage in fractured reservoirs.

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References:

Sojwal Manoorkar, Gülce Kalyoncu Pakkaner, Hamdi Omar, Soetkin Barbaix, Dominique Ceursters, Maxime Latinis, Stefanie Van Offenwert, and Tom Bultreys. From underground natural gas to hydrogen storage in fractured reservoir rock: comparing relative permeabilities for hydrogen versus methane and nitrogen. arXiv preprint arXiv:2411.14122, 2024

99

Multi-scale Reconstruction of Pore Networks Using Fully Connected Artificial Neural Network

Authors: Abolfazl Moslemipour¹; Saeid Sadeghnejad²

Co-authors: Frieder Enzmann³; Davood Khoozan⁴; Thorsten Schäfer²; Michael Kersten³

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Abstract

Digital Rock Physics (DRP) has become a useful tool for understanding rock properties [1]. However, modeling of heterogeneous rocks is challenging because of the trade-off between resolution and field of view [2, 3]. These rocks have complex porosities, making high-resolution imaging necessary but challenging at a large field of view. To address this, researchers have come up with multi-scale pore network modeling (PNM) and related reconstruction methods [4]. These methods capture images at different resolutions and integrate the extracted PNMs to create a unified multi-scale PNM. Industrial X-ray CT and FIB-SEM are common techniques for image acquisition in DRP. There are various methodologies that can be used to integrate PNMs from different resolutions and reconstruct a multi-scale PNM [5]. However, the reconstructed PNMs are often unrealistic and the integration process also fails to achieve sufficient accuracy. To address this challenge, we propose a solution by introducing a PNM integration approach for efficient multi-scale PNM reconstruction of rocks containing unresolved porosity. Our method separates resolved and unresolved porosities using different voxel sizes from CT scans at multiple resolutions. Resolved regions have larger voxel

sizes, while unresolved areas retain smaller voxel sizes. We suggest to extract macro-PNM from the resolved regions and generate stochastic micro-PNMs for the unresolved areas. A fully connected artificial neural network was developed to bridge between the micro- and macro-PNMs. The network was designed to predict the length and diameter of added throats between PNMs based on input data. Synchrotron CT images of Indiana limestone at two resolutions were used as the training dataset. Multi-scale PNMs were reconstructed for 10 different realizations. The permeability values of these PNMs were found to closely match laboratory-measured rock properties but not the porosity. The average porosity of the multi-scale PNMs thus reconstructed was $11.2 \pm 0.06\%$, compared to a laboratory-measured porosity of 18.9%. This difference is due to nano-scale pores that were not captured by the high-resolution imaging. However, these pores were observed to have a minimal impact on the rock's permeability. The average permeability of the multi-scale PNMs was determined to be 257 ± 3 mD, which aligned closely with the laboratory-measured value of 259 mD and demonstrated the accuracy of our multi-scale PNM reconstruction method.

Keywords:

Digital Rock Physics, Unresolved Porosity, Multi-scale Reconstruction, Pore Network Modeling, Artificial Neural Network

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Water & Porous Media Focused Abstracts:

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MS09 / 100

Analytical pore-scale modelling of the effect of particle surface roughness on the pressure drop and/or friction factor of granular porous media

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Surface roughness plays a critical role in modelling fluid flow parameters through granular porous media, with applications in, for instance, hydrology, thermal storage and biofiltration. Accurate flow prediction models are necessary for optimizing production and reducing capital costs. Over the years, the inclusion of surface roughness, defined as the microscopic irregularities on the surfaces of particles, have become apparent in many pressure drop model predictions. The importance of accounting for the effect of particle surface roughness on the pressure drop and/or friction factor of granular porous media has been highlighted by a few authors in the literature (e.g. Allen et al. (2013), Nemec and Levec (2005) and Crawford and Plumb (1986)). The two most common approaches include the use of fractal analysis or empirical modelling. In the case of the fractal modelling, it is often not as straightforward to quantify the fractal parameters. The empirical models, on the other hand, include curve fitting parameters which make these models data specific and not generally applicable, since for every other data set, new empirical coefficients need to be determined. In this study, an analytical pore-scale model is proposed for granular media involving the rectangular Representative Unit Cell (RUC) model (Du Plessis and Woudberg (2008)), which has served well in the literature. This granular RUC model is adapted geometrically to include particle surface roughness and the analytical modelling procedure for the derivation of the pressure gradient adapted accordingly. The resulting predictive equation includes a roughness factor, defined in terms of the average roughness height, amount of roughness elements and particle diameter. In fractal analysis models, the surface roughness is often represented as microscopic conical elements on the surface of granular media, where-as in this study it is represented as cubes, to comply with the rectangular geometry adopted by the RUC model. The proposed model is validated against experimental data from the literature involving flow of gas and/or water through smooth and rough granules. The well known Ergun equation (Ergun (1952)) for smooth particles is also included for comparison (and reference), as well as the empirical model of Allen et al. (2013) for smooth particles. The effect of roughness is, in addition, included into the latter model to, once again, illustrate the significant improvement in the model prediction with the inclusion of surface roughness. Results will furthermore be shown in which the RUC model has been applied to predict the pressure drop over a biofilter by taking particle surface roughness, sphericity and biofilm development into account. The findings of this study have the potential to improve the optimization of applications, such as biofiltration systems, and contribute to a deeper understanding of surface roughness characterization.

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Water & Porous Media Focused Abstracts:

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References:

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Relating oil-water two-phase flow pore-scale phenomenon to Darcy-scale constitutive relations

Authors: Avinoam Rabinovich¹; Avidan Ben-Shabat¹; Tianlei He²; David Weitz²

¹ *Tel Aviv University*

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Multiphase flow in porous media on large (Darcy) scales is conventionally modelled by constitutive relations: relative permeability and capillary pressure functions. These are typically obtained experimentally and are specific for a given porous medium and flowing phases under certain conditions. The approach, although widely used, is still under scrutiny. One of the fundamental challenges of modeling is how to interpret these constitutive relations in terms of pore scale fluid phenomenon. In this work we conducted an oil-water drainage experiment on a synthetic porous medium consisting of glass beads. The fluids and medium were visualized using confocal microscopy. We were able to characterize the saturation distribution in the porous medium both as a function of time at a specific location in the porous medium and throughout the entire medium at steady state conditions. We then characterized the constitutive relations by accurately matching a one-dimensional model to the transient results of the experiment. Insight is drawn regarding the relationship between the observed pore-scale flow and the resulting Darcy-scale relative permeability and capillary pressure functions.

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102

Upscaling CO₂-brine two-phase flow using deep neural networks

Author: Avinoam Rabinovich¹

Co-author: Subham Dhar¹

¹ *Tel Aviv University*

Corresponding Author: avinoamr@tauex.tau.ac.il

Modeling injection of CO₂ into brine aquifers for geological carbon storage is a crucial element of CCS projects. These models require the implementation of upscaling techniques, as most field scale models do. Upscaling of CO₂ injection into brine is challenging due to the significant fine-scale capillary heterogeneity phenomenon that is typically encountered and is then substantially reduced on the coarse scale, when using conventional upscaling methods. Upscaling using conventional methods can therefore lead to significant modeling errors. In recent years, heuristic methods have been explored for upscaling, including a number of publications suggesting machine learning based techniques.

We present an upscaling approach based on a two-step process. First, optimization is used to obtain upscaled properties: permeability, relative permeability and capillary pressure. This method leads

to an accurate match of coarse scale and fine-scale simulation results, however, it is expensive computationally and requires fully solving the fine-scale simulations. The second step involves training a deep neural network (DNN) model using the optimized upscaled properties calculated in the first step. The DNN upscaling model can then be used to upscale properties for similar flow conditions within a fraction of a second.

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MS08 / 103

Review of Chaotic Advection in Porous Media

Authors: David Mays¹; Roseanna Neupauer²

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Garrison Sposito's "Chaotic Solute Advection by Unsteady Groundwater Flow" (Water Resources Research, 42, W06D03, <https://doi.org/10.1029/2005WR004518>, 2006) was the first in a growing body of literature exploring chaotic advection in porous media. In the nearly two decades since, this literature has provided new insights into solute transport, mixing, and reaction across multiple scales, from the micrometer scale of pores to the 10-meter scale of groundwater remediation field sites, in two-dimensional (2D) and 3D geometries, including both natural and engineered flows, with contributions from groups in Australia, Canada, Germany, India, Spain, and the United States. In this presentation, we introduce this literature under the three headings of fundamentals, applications, and prospects. Starting with fundamentals, chaos refers to a deterministic system manifesting sensitive dependence on initial conditions, popularly known as the butterfly effect. This unpredictability results, not from inertial terms in the Navier-Stokes equations nor from random heterogeneity in the porous media, but from the nonlinear structure of the dynamic system itself. Chaotic advection refers to chaos in laminar flows, that is, flows at low Reynolds numbers that could result from high viscosity (for example in mixing paint or lava flows) or from small scales or low velocities (for example in micromachines). Chaotic advection in porous media generally includes small scales and low velocities but importantly, because porous media flows are generally irrotational, they exclude the mechanical stirrers employed in much of the broader literature on chaotic advection. Instead, chaotic advection in porous media refers to flows in which solute plumes are stretched and folded, popularly known as the baker's transformation. The analysis of such flows depends on Lagrangian analysis including Lyapunov exponents to quantify the butterfly effect and Poincaré sections to visualize the flow morphology. The literature features three principal applications to date, namely (1) ubiquitous chaotic advection at the pore scale, (2) naturally occurring chaotic advection at the Darcy scale, and (3) engineered chaotic advection, a subset of engineered injection and extraction (EIE). Among these applications, EIE has attracted the most attention so far, including theoretical developments, laboratory experiments, and one field test. Under prospects, these contributions lay the groundwork for future work under a broad conceptual framework in which porous media, both natural and engineered, serve as mixers and reactors despite the constraint of laminar flows. While the most popular application thus far has been groundwater remediation, chaotic advection in porous media also suggests promising applications for understanding natural processes, such as carbon and nutrient cycling, and engineered processes, such as in situ leach mining. In sum, if one begins with

the premise that the rich complexity of biogeochemistry is often transport-limited, then chaotic advection offers a conceptual framework to rethink flow as a knob that might be adjusted to overcome that limitation.

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MS17 / 104

Molecular investigation of pore size redistribution and formation deformation during the CH₄ displacement accompany with CCUS in shale under various influencing factors

Author: Jiawei Li¹

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The method of carbon dioxide (CO₂) injection in shale reservoirs has prevailed in recent decades, attributed to CO₂ injection promoting shale gas (CH₄) production while being sequestered to eliminate the greenhouse effect for an environmentally friendly society. However, the efficiency of CO₂-enhanced CH₄ recovery (CO₂-EGR) in shale reservoirs is influenced by geological factors, including depth-induced variation in temperature and pressure and subsurface water encroachment with various salinity. The CO₂-EGR process induces pore size redistribution and formation deformation, which is attributed to the reaction of CO₂ adsorption and CH₄ desorption from the surface of the shale slit and tiny pores inside the matrix. Meanwhile, this reaction, in turn, affects the CO₂-EGR performance owing to the variation in the physical characteristics of shale. In order to reveal the fundamental mechanisms of the CO₂-EGR to develop a high displacement efficiency, as well as the formation dynamic response for the CO₂-EGR process, a hybrid simulation method of molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) process is carried out to uncover the gas adsorption and displacement from a molecular aspect. The molecular dynamics can be established at various temperatures and pressures, and other geological factors can be quantified and added into the simulation system, which is an effort-saving and visualization-friendly way. Adsorbed gas is primarily present in the organic matter of shale, and the adsorbed gas positively relates to the organic carbon content, owing to the large specific surface area and significant pore volume. Therefore, this study employs the type II-D kerogen fragment (C₁₇₅H₁₀₂N₄O₉S₂) to construct the flexible shale matrix. This work observes that, for pure gas adsorption, CH₄ increases by 9.2% at 308 K, 10.8% at 338 K, and 11.9% at 368 K in the deformable model than that of the fixed one. In contrast, CO₂ has a 36.5% increase at 308 K, a 39.3% increase at 338 K, and a 44.4% increase at 368 K, presenting that the flexible model preserves additional CH₄ and sequesters more CO₂ than estimated. Subsurface water is also added at 0-5 wt% of the organic model with the salinity of 3-6 mol/L NaCl solution. Moisture has a noticeable pore space reduction effect, and 5 wt% moisture content leads to a 44.9% reduction in CH₄ adsorption, compared to a 24.5% reduction in CO₂ adsorption. Moreover, the 6 mol/L NaCl within 5 wt% moisture content further reduces CH₄ adsorption by 9.8%, compared to 13.8% for CO₂. Subsurface water suggests an impeded influence on CH₄ adsorption and CO₂ sequestration.

The preferential selectivity SCO_2/CH_4 , as a competitive determination and displacement indicator, is addressed for the equimolar binary mixture between CO_2 and CH_4 under the above influencing factors and observes moisture positively influences SCO_2/CH_4 , salinity promotes SCO_2/CH_4 , and C_2H_6 develops SCO_2/CH_4 . This study sheds light on the CO_2 -EGR project and advances the CCUS in unconventional reservoirs.

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Poster / 105

Case study for determination of safety mud window and analysis of fluid characteristics for wellbore stability in shale by coupling THMC method

Author: Hailei Sun¹

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During drilling, the instability of the wellbore is always a severe problem, which might lead to borehole failure in shale formation. But this kind of borehole failure could be eased using the optimum mud weight and the better well trajectory. Many drilling problems include the kick or blowout, wellbore collapse, or lost circulation. This study applied a geo-mechanical model and rock failure criteria to the wellbore stability analysis to determine the safety mud weight. The numerical simulation was conducted using MATLAB. A rock-fluid coupled model was also solved using the finite element method under the ABAQUS framework, and the results were compared with those of the uncoupled model. This work would support solid foundation in wellbore stability during the drilling process, and would shed the light in computing the safety mud weight in high accuracy.

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CO₂ trapping efficiency and geo-mechanical risks associated with geological carbon storage in continental flood basalts

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Continental Flood Basalts (CFBs) have recently garnered significant attention as a prospective target for geological carbon storage (GCS) due to their vast areal extent, good hydraulic connectivity, and mineralogical composition conducive to trapping CO₂ as stable secondary carbonates. However, understanding the complete feasibility of CFBs for GCS requires further studies due to the complexities associated with carbon trapping. Unlike conventional siliciclastic formations, the potential injection intervals of CFBs consist of interbedded vesicular zones. Vesicular intervals range in thickness from a few meters to tens of meters and the pore network properties (range in pore size and pore connectivity) are highly variable. This heterogeneity results in greater uncertainty in the prediction of the CO₂ plume extent, the CO₂ trapping efficiency and pressure build-up during industrial-scale CO₂ injection.

This study highlights the trapping efficiency and geo-mechanical risks associated with injecting CO₂ in form of supercritical CO₂ (sc-CO₂) and CO₂-enriched water (CO₂-ew) in CFBs. Two 3D reservoir domains (4 meters and 10 meters thick) representing vesicular basalt layers were developed. A range of geological and multiphase flow properties was used to model scenarios that varied from well- to poorly-connected systems. The Van Genuchten-Mualem and Van Genuchten equations were employed to model the effects of relative permeability and capillary pressure. Injection of sc-CO₂ and CO₂-ew was simulated at three different rates (100 ktpa, 500 ktpa, and 1 mtpa), resulting in a total of 90 simulations. A range of in-situ stress field conditions—spanning normal fault, strike-slip fault, and reverse fault regimes under different tectonic stresses—were analysed to assess their impact on potential rock failure. The Mohr circle, Mohr-Coulomb, and Griffith criteria were utilized to visualize changes in the state of stress.

Our results demonstrated that pore fluid pressure began to increase within approximately one day of injection, with higher pressure buildup observed in sc-CO₂ injection scenarios. The thinner domain (4 meters) was found to be geo-mechanically less suitable for efficient injection of both sc-CO₂ and CO₂-ew phases, particularly at higher injection rates, due to its limited capacity to dissipate pressure. However, limited reservoir thickness was associated with higher pore space utilization (34.4%) at lower injection rates (100 ktpa) compared to the thicker domain (15.8%) (Figure 1a). Notably, some models at higher injection rates (500 ktpa) showed up to 90% pore space utilization for the thinner domain. Conversely, the thicker vesicular domain (10 meters) proved to be better suited for efficient injection of both sc-CO₂ and CO₂-ew phases in terms of geo-mechanical stability. Moreover, thrust fault regimes under moderate tectonic stress conditions provided more stable environments for CO₂ injection (Figure 1b, c), thereby minimizing the likelihood of geo-mechanical failure.

Figure 1: (a) Comparison of pore space utilization in the first (4 meters) and second (10 meters) domain for 100 ktpa injection. Comparison of geo-mechanical failure analyses for the second domain for (b) sc-CO₂ and (c) CO₂-ew injections under moderate (left panel) and extreme (right panel) tectonic stress in thrust fault regimes.

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An innovative diagnostic methodology to optimize brine composition in a LSWF process from laboratory experiments

Authors: Jesus Manuel Carmona Perez¹; MARTIN A. DIAZ-VIERA¹

Co-authors: Bernardo Carreón-Calderón¹; Enrique Serrano-Saldaña¹

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In recent years, there has been considerable interest in low salinity water flooding (LSWF) as an enhanced oil recovery (EOR) technique, which represents a viable and economically feasible alternative to conventional methods for carbonate reservoirs. A key problem with much of the literature regarding LSWF is that existing approaches to calculate oil recovery require laborious laboratory investigations, resulting in significant time and financial investment.

The aim of this work is to present an innovative diagnostic methodology for optimizing brine composition in a LSWF process from laboratory experiments by quantifying wettability alterations through the Bond Product Sum (BPS) index, which measures the electrostatic interaction forces between oil-brine and rock-brine interfaces.

The proposed methodology consists of two stages. First, the BPS is obtained by the chemical equilibrium of the interaction between brine, oil and rock by minimizing the Gibbs free energy in a process where the brine salinity is altered. Second, the relative permeability curves are calculated by an invasive percolation approach using a pore network model from laboratory data of interfacial tension and contact angle.

The methodology was applied to a case study of a spontaneous imbibition experiment in a Bedford limestone sample with a reservoir oil and brines with different compositions. The resulting correlations between BPS and oil recovery values are interpreted by modifying the relative permeability curves as a possible diagnostic tool for the viability of the LSWF enhanced recovery process.

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Poster / 108

Impact of Biotic Reactions on Hydrodynamics of UHS: A Pore-Scale Study

Author: Aruzhan Tleubek¹

Co-authors: Arvand Vedadi¹; Amin Hamed Mashhadzade¹; Salah A Faroughi¹

¹ *University of Utah*

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Hydrogen has emerged as a promising alternative for sustainable energy and plays a pivotal role in the transition from fossil fuels to green energy. With this growing reliance on hydrogen, the demand for efficient and scalable energy storage solutions has become increasingly critical. Among the various methods available, underground hydrogen storage (UHS) stands out as a cost-effective solution for long-term, large-scale energy storage. UHS involves injecting hydrogen into geological subsurface formations, including depleted hydrocarbon reservoirs, salt caverns, and saline aquifers. However, a major challenge in UHS arises from the activity of subsurface microorganisms, such as methanogens, sulfate-reducing bacteria (SRB), and acetogens. These microorganisms use hydrogen as an electron donor, producing impurities such as methane (CH₄) through methanogenesis, hydrogen sulfide (H₂S) through reduction of sulfate, and acetic acid (CH₃COOH) during acetogenesis. Microbial activities within porous media thus profoundly affect the hydrodynamics of the system and induce alterations in its physical properties, which can impact storage efficiency and hydrogen recovery. Despite experimental efforts to study these effects at the pore-scale, the results remain inconsistent, and simulations, on a larger scale, that account for microbially induced impurities are also very limited. Therefore, evaluating the biotic effects on the hydrodynamics of UHS is essential to understand the risks associated with the hydrogen loss and recovery rate in these systems.

This study addresses these knowledge gaps by conducting pore-scale analysis to investigate the hydrodynamics of UHS systems under realistic storage conditions, focusing on the behavior of rock-hydrogen-brine interactions during the cyclic injection, storage, and withdrawal phases in the presence of methanogens and SRBs. Our pore-scale analyses are employed to model the effects of microbial metabolisms on wettability, hydrogen diffusion, and relative hydrogen permeability. Microbial products are introduced during the storage stage and their impact is analyzed throughout the storage and withdrawal phases of UHS. The results demonstrate that the presence of microbial-mediated impurities causes the rock surface to slightly alter in terms of wettability, which can greatly influence fluid-rock interactions and dynamics. We also report that hydrogen diffusion decreases with increasing concentrations of microbial impurities. Furthermore, the shift in wettability and reduced hydrogen mobility, in turn, impact the relative permeability of hydrogen, highlighting the importance of microbially-induced changes on storage efficiency and recovery dynamics in UHS systems. Our findings provide critical insights into optimizing UHS designs to mitigate biotic impacts.

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Microscopic Mass Transfer Mechanism of Oil Recovery Coupling Displacement and Imbibition in Matrices and Fractures with Different Pore-Throat Structures

Author: Binyu Wang¹

Co-authors: Renyi Cao ¹; Gaofei Yan ¹; Linsong Cheng ¹; Jiangpeng Hu ¹; Huangchen Ren ¹

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Displacement-imbibition coupling oil production is a critical technique for enhancing oil recovery (EOR) during water injection development in tight/shale reservoirs. However, the role of pore-throat structures in reservoir rocks during displacement-imbibition processes and their impact on microscopic mechanisms and flow dynamics at different pore scales remain unclear. This study integrates pore-scale numerical simulations and core-scale nuclear magnetic resonance (NMR) experiments to monitor the entire migration process of oil and water phases. The microscopic utilization characteristics and influencing factors of pores at various scales are quantitatively investigated. The results indicate that displacement-imbibition coupling oil production, driven by multiple driving forces (displacement and imbibition interactions), effectively achieves balanced utilization across pores of different scales, making it a superior EOR method. The key mechanisms of displacement-imbibition coupling oil production involve pressure oscillation and capillary imbibition. By artificially altering the pressure field within the matrix pores, pressure oscillations between pores are induced, enhancing the capillary imbibition effect, reducing the utilization threshold of pore throats, and promoting oil recovery. The pore-throat structure of rocks determines the effectiveness of displacement-imbibition coupling oil production. Rocks with higher heterogeneity and better pore-throat connectivity reduce resistance to oil and water movement, enabling more effective utilization of the coupling mechanism and improving pore-scale recovery efficiency. Additionally, the complexity of matrix-fracture interactions significantly affects fluid exchange during the displacement-imbibition process. More complex contact relationships between the matrix and fractures result in a larger contact area, facilitating the displacement of oil droplets from pore spaces and enhancing imbibition between the matrix and fractures while weakening displacement effect. These findings provide theoretical insights into the mechanism of displacement-imbibition coupling oil production between the matrix and fractures and offer guidance for the efficient development of tight/shale oil reservoirs.

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Poster / 112

Impact of Particle Shape on Permeability in Unconsolidated Sandstone: Implication from Synthetic Models of Digital Rock Physics

Author: Katsumo Takabayashi¹

Co-author: Yasutaka Iijima ¹

¹ *INPEX CORPORATION*

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Our research team is devoted to developing rock property acquisition techniques for CO₂ sequestration projects in shallow aquifers. Target reservoir depth of CCS (Carbon Capture and Storage) in aquifers can be shallower than the most of E&P project in terms of economic efficiency. It infers that CCS projects have more chance to deal with unconsolidated rocks. Evaluating unconsolidated rocks is sometimes difficult, because there is uncertainty in acquisition of rock cores through drilling, which may result in lack of direct measurement of rock properties. To overcome this obstacle, we employed Digital Rock Physics (DRP) technology, which is indirect evaluative methodology applied for target reservoir. We created a digital model of the porous media simulating the reservoir rocks by packing objects that mimic sand particles. This synthetic digital model allowed us to calculate the permeability, which is a parameter indicative of the ease of fluid flow and essential for determining CO₂ storage capacity.

In this study, we examined effect of particle shape on permeability. As parameters representing particle shape, circularity and aspect ratio of sand taken from the outcrop were measured. The aspect ratio of 0.7 and circularity of 0.917 were used for the models. Three types of particles model were prepared: sphere, ellipsoid, and Nonspherical Irregularly Shaped Particles (NISP). Ellipsoid model reflects aspect ratio, and NISP model reflects both aspect ratio and circularity. All three models reflect the particle size distribution measured by the sieve method.

Higher permeability was calculated with the model filled with sphere particle compared with the other two models. The calculated permeability of the ellipsoid and NISP models were close. It is interpreted that there is no significant difference between the ellipsoid and NISP models, which infers that the aspect ratio is the main control parameter for permeability in this case.

A sensitivity study was conducted on the aspect ratio and circularity to investigate effect of particle size on relationship between permeability and porosity. 15 ellipsoid models were created by changing the aspect ratio from 0.3 to 1.0. It is found out that the increase in permeability relative to the increase in porosity is smaller when aspect ratio is close to 1.0. Next, 144 NISP models were created with 32 circularity ranging from 0.81 to 0.98. The increase in permeability against increasing porosity tended to slow down with decreasing circularity. However, the relationship was not as clear as at aspect ratio.

Finally, a revised ellipsoid model was created by using high resolution particle size distribution. The calculated permeability was compared to measured permeability and found out that these permeabilities were within the same error range with previous studies which targeted consolidated sandstone. As a result, the permeability of unconsolidated sandstone was successfully estimated using the synthetic digital model with high resolution particle size distribution.

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Pore-scale study of mineral reactions in the near-wellbore region for CO₂ storage in Deep Saline aquifers

Author: Qigui Wang¹

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Abstract: The study of CO₂ dissolution effects on rock reservoirs during CO₂ storage and CO₂-enhanced oil and gas recovery is crucial for the effectiveness of underground carbon sequestration projects and for improving oil and gas recovery rates. In this study, the Darcy-Brinkman-Stokes (DBS) model is used to model the reaction-transport at the rock pore scale, based on the theory of microscopic continuous media, and solved discretely using COMSOL, a coupled Multiphysics field simulation software, to investigate the dissolution reactions and the evolution of the porous medium during carbon sequestration. The model elucidates the nonlinear coupling inherent to the mineral dissolution process, offering insights into the intricate interactions between seepage, solute transport, and reaction fluid chemistry. The findings indicate that soluble minerals are progressively dissolved over time, leading to the formation of new seepage channels and a consequent reduction in the dissolution rate within the original seepage channels. An increase in formation water salinity results in a reduction in solution pH, which in turn affects the chemistry of reservoir minerals. Conversely, an increase in reservoir temperature, pressure, and injection rate promotes calcite dissolution. Furthermore, the augmented pressure differential propels the expansion of the reaction zone towards the midstream, thereby accelerating the dissolution and reaction process of calcite nodes. These findings provide a theoretical foundation for future carbon capture and storage technologies. **Key words:** gas-water two-phase seepage, multiphase dissolution, multiphase interface evolution, mass transfer and diffusion, and chemical reaction dynamics.

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MS20 / 114

Impacts of Biofilms on Microplastics Movement and Aggregation

Author: Guanju(William) Wei¹

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Microplastics pose significant environmental and health challenges due to their widespread presence in aquatic systems and their potential for ingestion by animals and humans. While much research has focused on the transport of microplastics, the role of biofilms in modulating microplastic transport remains underexplored. Most studies conclude that biofilms decrease microplastic transport. Here, we demonstrate that biofilms can also increase microplastic transport under certain conditions through a combination of microfluidic experiments, confocal imaging, numerical simulations, and theoretical models. We seeded a straight microfluidic channel with polystyrene microspheres and injected *Pseudomonas aeruginosa* solution into the channel. We observed that biofilms developed on the surfaces of microplastics of certain sizes under certain shear stress conditions. Furthermore, we discovered that such biofilms can reduce the critical shear stress required for beads movement by an order of magnitude. By simulating the flow field around biofilm-coated beads, we revealed that such biofilms facilitated microplastic movement by increasing both drag and lift forces. In addition to colonizing microplastic surfaces, we found that biofilms can promote the formation of aggregates

by altering the trajectories of these microplastic beads, thereby increasing their encounter rate. In summary, our results demonstrate that biofilms can enhance the transport of microplastics of certain sizes as well as promote the formation of particle clusters. Our findings underscore the significant influence of biofilms on microplastic transport and aggregation and have implications for predicting and mitigating microplastic pollution.

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MS08 / 115

Solute mixing in Darcy-scale heterogeneous porous media: stochastic and interacting dispersive lamellae

Author: Aronne Dell'Oca¹

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We investigate the mixing dynamics of a large solute plume transported by advection and local diffusion in Darcy-scale porous formations characterized by randomly heterogeneous distributions of hydraulic conductivity. We test the dispersive lamella mixing model for mildly to highly heterogeneous formations. At the core of the dispersive lamella mixing model lays a single non-interacting transport Green function that dilutes according to the effective dispersive scale. This picture falls short in highly heterogeneous formations. Thus, we extend the mixing model to account for the heterogeneity-induced (i) variability in the dispersive behaviors of distinct lamellae (or transport Green functions) and (ii) their interactions. In particular, we relate the latter to the occurrence of strong flow focusing in highly heterogeneous formations and we identify key dispersion-related scales that capture the impact of small and large lamellae interactions on the dynamics of solute mixing.

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MS04 / 116

Swelling Porous Media –The Effect of Swelling Pressure on Modeling Flow and Wave Propagation**Author:** Lynn Schreyer¹**Co-authors:** Ryan Whitehead²; Pratap Sahay³; Keith Wojciechowski⁴¹ *Washington State University*² *Washington State University Math Department*³ *Centro de Investigacion Cientifica y de Educacion Superior de Ensenada*⁴ *University of Wisconsin-Stout***Corresponding Authors:** lynn.schreyer@wsu.edu, pratap@cicese.edu.mx, ryan.j.whitehead@wsu.edu, wojciechowskik@uwstout.edu

The ability of a saturated swelling porous medium to swell can be measured using a reverse osmotic swelling experiment [3]. This experiment demonstrates that the liquid pressure inside a swelling porous medium (termed vicinal fluid) is different from that of fluid outside the porous medium in equilibrium with it (termed bulk fluid), and this in turn affects the flow of fluid and the speed of pressure waves. Here we use hybrid mixture theory to show how swelling pressure affects flow and swelling [1,5], and how it also affects the speed of pressure waves (Biot wave equations [2]), typically used to determine material properties. For flow, the classical Darcy's law incorporates additional terms involving the gradient of porosity [1], and we illustrate an application by modeling a swelling polymer used for drug delivery such as Aleve [5]. For wave propagation the speed is modified by the swelling pressure and its significance is determined by the ratio of the swelling pressure and the P-wave modulus. Thus for soft swelling materials, the pressure wave speeds are significantly impacted, influencing e.g. the measurement of material parameters using pressure wave speeds [4].

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Poster / 117

Dynamics of pore-scale protean droplets in porous media

Authors: David Meer¹; Shivnag Sista²; Corey O'Hern²; Mark Shattuck³; Eric Weeks¹

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² *Yale University*

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We study a quasi-2D oil-in-water emulsion flowing through a microfluidic porous material, stabilized into droplets by a weak surfactant. The porous material creates droplet breakup against static obstacles, and the weak surfactant does not completely inhibit coalescence. Therefore, the droplets arrive at a steady-state size distribution, which is a function of the system geometry, flow speeds, and fluid properties. We show how parameters like capillary number, deformation, and collision symmetries, and relative positions of neighboring droplets relate to breakup and coalescence probabilities, and how the breakup and coalescence chances create our steady-state size distribution.

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MS26 / 118

CO2 Geological Storage Modeling with Machine Learning

Author: Gege Wen¹

Co-authors: Isaac Ju²; Sally Benson²

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CO2 geological storage plays an essential role in global decarbonization and the energy transition. Predicting the transport of CO2 in subsurface formations requires numerical simulations of multi-phase flow through porous media. However, such simulations are challenging at scale due to the

high computational costs of existing numerical methods. As a result, the lack of efficient modeling approaches can lead to significant uncertainties in evaluating storage capacities and optimizing for safe and effective injection sites.

Machine learning (ML) provides a powerful alternative to numerical simulation with several orders of magnitude speedups while maintaining comparable accuracy. We demonstrate the viability of a general-purpose ML-based framework that can serve as an alternative to numerical simulation for modeling CO₂ geological storage through a series of progressively more powerful ML model architectures, including convolutional neural networks, enhanced-Fourier Neural Operators (U-FNO), Nested Fourier Neural Operator (FNO), and graph neural operators (MGN). The ML modeling series provides predicting capabilities across reservoir and basin scales, speeding up flow prediction up to 700,000 times compared to numerical methods.

The fast inference of machine learning models enables many critical tasks for CO₂ geological storage decision-making that were prohibitively expensive. This framework allows for unprecedented real-time modeling and probabilistic simulations that can support the scale-up of global CO₂ geological storage deployment. The trained machine learning models are hosted in the public web application <https://CCSNet.ai> to demonstrate the predictability to the community.

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MS24 / 119

Adsorption-Induced Deformation and Its Impact on Gas Transport in Microporous Coal Matrix

Authors: Quanlin Yang¹; Zhehui Jin¹

¹ *University of Alberta*

Corresponding Authors: jinzhehui25@hotmail.com, zhehui2@ualberta.ca

Adsorption-induced deformation in microporous coal matrix has been largely overlooked in gas transport studies, despite its significant influences on pore geometry and diffusive pathways. In this work, we employ a hybrid grand canonical Monte Carlo (GCMC) and molecular dynamics (MD) scheme under various loading conditions to capture both gas adsorption and matrix deformation behavior. Equilibrium MD simulations are then performed to quantify CH₄ and CO₂ self-diffusivity. Results show that deformation enhances adsorption, with CO₂ displaying greater uptake and volumetric strain than CH₄. A universal linear relationship among gas loading, free volume ratio, and self-diffusion coefficients holds for both rigid and flexible matrices, but with a gentler slope in flexible matrices—indicating reduced diffusion sensitivity to diminishing free volume at higher loadings. Geometrical and effective tortuosity variations reveal that strong CO₂ adsorption induces significant swelling and complex matrix rearrangements at elevated loadings, pushing geometrical tortuosity (~3.70) well beyond rigid-matrix levels (~2.49), while weak CH₄ adsorption produces milder, more uniform adjustments on matrix geometrical tortuosity (from ~2.80 down to ~2.40). Consistent drop in effective tortuosity across all cases indicates that gas motion is increasingly hindered by neighboring molecules, rather than gas-solid interactions. Overall, our findings clarify how gas adsorption,

matrix deformation, and self-diffusivity co-evolve in microporous coal matrix, and provide important guidance into enhanced gas recovery and CO₂ sequestration that require accurate transport modeling in deformable media.

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Canada

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MS13 / 120

Microscopic Origin of Hysteresis in CH₄ Sorption-Induced Deformed Coal Matrix: Insights from Stepwise Hybrid GCMC/MD Simulations

Authors: Quanlin Yang¹; Zhehui Jin¹

¹ *University of Alberta*

Corresponding Author: zhehui2@ualberta.ca

CH₄ sorption hysteresis is pivotal for predicting coalbed methane (CBM) production, yet its driving factor—the coupling of gas sorption and coal deformation—remains incompletely understood. Here, we use a stepwise hybrid grand canonical Monte Carlo/molecular dynamics (GCMC/MD) simulation technique to track continuous CH₄ adsorption and desorption in a deformable coal matrix. Both matrix internal rearrangement and swelling contribute to pronounced sorption hysteresis and pore structure hysteresis. At the same chemical potential, pore size distribution and 3D pore space visualizations clearly show that the matrix fails to revert to its original configuration upon unloading, indicating structural irreversibility. Using free energy perturbation (FEP) method, we compare the free energy difference required to detach adsorbed gas (the energy barrier) and find that CH₄ remains more strongly confined in local energy minima on the desorption path, even at lower loadings, leading to consistently higher free energy difference values (200–237 kBT) than on the adsorption path (165–225 kBT). These findings underscore how irreversible matrix rearrangements and deeper local minima along the desorption route drive persistent sorption hysteresis. Overall, our results highlight the necessity of incorporating sorption-induced deformation and structural hysteresis into predictive models of gas transport and storage in deformable coal.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

MS10 / 121

Controlling ice formation at the interface between a solid and a liquid in view of nano-scale imaging resolution

Author: Alberto Guadagnini¹

Co-authors: Chiara Recalcati ; Gianlorenzo Bussetti ¹; Lamberto Duò ¹; Monica Riva ¹; Rossella Yivlialin ¹

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We provide an original experimental approach to induce controlled freezing and thawing at a solid-liquid interface in view of imaging the process at nano-scale resolution. The study is framed in the broad context of the assessment of the key drivers promoting ice formation in the presence of a substrate such as minerals. In this sense, observing and quantifying formation and behavior of ice at solid-liquid interfaces is a critical research area. It bears significant implications in, e.g., geochemistry (in the context of chemical and mechanical weathering of rocks), climate science (with reference to the formation of ice on mineral dust in the atmosphere and permafrost thawing), or cryobiology (to optimize applications such as cryopreservation or unravel adaptation dynamics of microorganisms such as bacteria to extreme conditions). Traditional experimental techniques to analyze ice nucleation chiefly rely on exposing pre-cooled substrates to humid vapors. Doing so typically limits precision and control over key variables in interfacial studies. Our original experimental approach is specifically designed to overcome these limitations. We rely on Highly Oriented Pyrolytic Graphite (HOPG) as a model substrate and document controlled freezing. The latter is obtained by periodically cooling the interfacial layer while maintaining the bulk liquid water at a stable temperature above 0 °C. Nano-scale resolution imaging is obtained through Atomic Force Microscopy. Our experimental design enables us to achieve an accurate temperature control (about ± 0.1 °C). This, in turn, allows minimizing drift issues during surface scans. We outline the design of our experimental set-up and the key elements of our unique combination of experimental methodologies. We then provide perspectives about broader implications of our findings to advance porous media science upon encompassing the effects of ice nucleation dynamics and interfacial processes on the structure of complex pore spaces.

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References:

122

Imaging-based Dispersion in Flow Experiments with 4D Imaging

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Experiments in porous media make increasingly use of 3D imaging technology. While initially 3D imaging was mainly used to assess rock heterogeneity in a qualitative manner, over the past decades the imaging technology has matured to acquiring time series of 3D images (“4D”) in-situ during flow experiments. Examples range from imaging of tracer tests in natural rock to assess heterogeneity, tracking immiscible displacement processes in hydrocarbon recovery, CO₂ sequestration and underground hydrogen storage, respective trapping patterns, hydrate formation, and providing in-situ saturation profiles for determining relative permeability and capillary pressure, to transport processes in technical porous media such as fuel cells, batteries and other electro-catalytical devices.

The X-ray computed tomography methods (but also other 3D imaging techniques) commonly used for this purpose have a finite acquisition time. Depending on the flow velocity, this scanning time may not be negligible in relation to propagation of concentration / saturation distribution within the porous medium. As it occurs in photography of relatively fast-moving objects where a long shutter time will lead a “motion blurring”, similar effects can occur in core flooding experiment because of the relative movement of the concentration plum and the imaging system. This “image dispersion” or blurring can then be mis-interpreted as physical (hydrodynamic) dispersion.

To demonstrate the impact, we consider the scenario of solute transport. For illustration purpose we start with a 1D dispersive example where the degree of image-dispersion on the concentration profiles comes as an additional smearing of the profiles as the relative velocity of the CT imaging to the fluid front increases. We then proceed with 3D scenarios where it is demonstrated how imaging-based dispersion leads to the misinterpretation of flow in spatially resolved heterogeneity as hydrodynamic dispersion.

The findings suggest that the imaging-based dispersion effect needs to be considered for practically all 4D imaging methods such as CT, PET, MRI of dynamic processes with respect to the interpretation of heterogeneity and its effects, e.g. hydrodynamic dispersion, capillary dispersion of a flow front.

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MS06-B / 123

Statistical scaling of nanoscale spatially heterogeneous dissolution rates at mineral-water interfaces

Author: Chiara Recalcati^{None}

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Dissolution and precipitation processes taking place at the interface between water and the solid matrix of the host porous medium are key drivers for chemical weathering of minerals in subsurface

environments. Direct high-resolution imaging of mineral substrates subject to dissolution/ precipitation document that these reactions are driven by local mechanistic phenomena originating at natural defects embedded in the mineral lattice. These are typically viewed as randomly distributed across the mineral system and constitute a major element imprinting the pattern associated with the dynamic self-organization of the water-mineral interface. While their presence triggers the formation of characteristic interfacial patterns starting from the nanoscale, their action manifests across diverse spatial scales. It ultimately yields starkly heterogeneous distributions of reaction rates that can display several-fold variations across the same mineral surface. Sample probability density functions of mineral dissolution rates are documented to display complex non-Gaussian behavior. When homogenized across a given window of observation on a crystal surface, these distributions are characterized by multiple modes. These are, in turn, linked to mechanistic processes driving the reaction. Advancing our fundamental understanding and modeling capabilities of environmental scenarios underpinned by chemical weathering processes (including, e.g., carbon sequestration, pollutant migration/stabilization, or fracture morphology dynamics) requires incorporating spatial heterogeneity of reaction rates into reactive transport models. This spatial heterogeneity, which fundamentally originates at the nanoscale, plays a critical role in shaping system behavior. Accurately capturing and representing the statistical characteristics associated with these nanoscale variations within modeling frameworks is key for improving model results and fostering robust interpretations of these complex environmental phenomena.

In this broad context, understanding and providing a sound representation of the way in which key traits emerging from stochastic analysis of data transition with scale is a major research aspect. Here, we focus on calcite-water interfaces as a model geochemical system. We consider nanoscale spatial distributions of dissolution rates obtained from Atomic Force Microscopy measurements of the topography of a calcite sample subject to dissolution under continuous flow conditions. We investigate the scaling behavior of the ensuing random fields upon analyzing sample structure functions. The latter correspond to absolute q -th order statistical moments of spatial increments (i.e., differences between values of observed dissolution rates taken between two locations separated by a given distance or lag). Our analyses document that dissolution rates exhibit two distinct power-law scaling regimes. These are in turn associated with diverse degrees of persistence, as rendered through the classical Hurst exponent. We then provide a direct link between the occurrence of such regimes and the nanoscale mechanistic processes driving the evolution of the mineral-water interface.

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Poster / 124

Modelling Anomalies in Non-Ideal Gas Dispersion during Underground Hydrogen Storage

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Gas displacement in porous media is a vital process with broad industrial and environmental applications. A prominent example is underground hydrogen storage, where understanding the interaction

and mixing of hydrogen with cushion gas is essential. This study investigates irregularities in the dispersion behaviour of gas mixtures during opposing flow scenarios, specifically injection and production, from a modelling perspective. Compared to Newtonian fluids, the gaseous nature of the system introduces significant challenges, including non-ideal mixing, compressibility, and higher diffusivity. The results reveal distinct dispersion patterns between injection and production, with increased non-ideality in the gas mixture intensifying these discrepancies. Unlike dispersivity observed in Newtonian fluids within porous media, this research demonstrates that gas displacement dispersivity is influenced not only by the properties of the porous medium but also by the characteristics of the gaseous components.

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MS26 / 127

Improving CO₂ Injectivity with Surfactant-Driven Methods in Geological Storage

Author: Yeon-Kyeong Lee¹

Co-authors: Yong-Chan Park¹; Kue-Young Kim¹; Joo Yong Lee¹; Gidon Han¹; Min-Kyung Jeon¹; Chan Hee Kim¹

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Injectivity is an important factor in the carbon dioxide (CO₂) geological storage, as it determines how quickly and efficiently CO₂ can be injected into underground reservoirs. Improved injectivity not only enables more effective use of storage space but also makes it easier and more cost-efficient to store CO₂ in challenging reservoirs. Surfactants, which have both hydrophilic and hydrophobic components, can significantly alter the rocks and fluids interactions. They reduce the interfacial tension between CO₂ and brine and modify the wettability of rock surfaces, facilitating CO₂ flow through smaller pores. To investigate these effects, detailed experiments were conducted, including measurements of interfacial tension and contact angles under varying conditions such as different surfactant types, temperatures, and pressures. Utilizing a synchrotron-based 3D computed tomography (CT) scanner, advanced imaging techniques were also employed to visualize CO₂ flow dynamics at the pore scale during injection. At the core scale, multiphase fluid flooding experiments were performed to measure saturation and relative permeability using 2D X-ray imaging equipment. These experimental results demonstrated that surfactants can increase CO₂ saturation and relative permeability while significantly reducing injection pressure, thereby improving injectivity. These findings highlight the potential of surfactant-based methods to optimize CO₂ injectivity, contributing to more effective and economical geological storage solutions.

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MS09 / 128

Improved stochastic pore network generation algorithms for porous media

Author: Chengnan Shi¹

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Pore-scale modeling and simulation are widely applied to investigate transport phenomena in porous media. Because the applicability of direct methods, like lattice Boltzmann and particle-based methods, remains restricted due to their high computational cost, pore network modeling (PNM) has emerged as one of the most efficient and effective approaches for practical applications. However, the direct extraction of a full pore network (PN) from 3D pore structure images is often infeasible for materials with wider pore size distributions, owing to the inherent conflict between image resolution and field of view. Therefore, achieving representative and reliable PNs often necessitates both scale-extension (expanding small actual networks to large virtual networks) and scale-integration (merging multiple single-scale PNs as extracted from single 3D images).

Given the stochastic nature of pore structures in porous media, scale-extension and scale-integration are typically accomplished through stochastic PN generation. After extracting the template PN from a 3D image, its geometrical and topological features are translated into statistical information, which is then used to generate the desired PN at arbitrary size. The generated PN is statistically equivalent to the extracted PN, by retaining its key geometric and topologic characteristics. In this study, three existing geometry replica algorithms (G_1 to G_3) from the literature are implemented, along with the proposed improved G_4. G_4 targets the porosity-weighted pore radius distribution and also employs stratified random sampling to determine geometric PN parameters. These parameters are obtained through a Gaussian multivariate copula that integrates marginal probability distributions with joint correlations. Additionally, two improved topology replica algorithms T_1 and T_2 are put forward. T_1 uses a quasi-random low-discrepancy Sobol sequence to determine the location of the pore bodies, while T_2 examines the ranges of neighboring pores considered for pore body connection.

These stochastic algorithms are evaluated by comparing simulated unsaturated hygric properties of generated PNs with those of the extracted PNs. Ten PNs are generated for each algorithm to ensure robust results, and a PN-based hygric property simulator is employed to attain the moisture retention and permeability curves, as storage and transport property respectively. The resulting curves are first assessed visually for qualitative comparison, which is followed up by a quantitative evaluation using four deviation indices. To demonstrate the exhaustive effectiveness and adaptability of the improved algorithms, PNs from four porous materials, with varying degrees of complexity, are applied: Ketton carbonate, sintered glass, Berea sandstone and ceramic brick.

The results reveal that the combination of G_4 and T_2.3 –where the number of neighboring pores considered for connections is five times the maximal coordination number of the extracted PN – highly enhances the reliability of the generated PNs. Compared to the basic geometry and topology replica algorithms, the deviation indices are relatively reduced by an average of 67% to 98%.

These improved stochastic algorithms for single-scale PNs also pave the way for generating full-scale PNs of porous materials with exceptionally wide pore size ranges. Future research can build on these algorithms to generate such full-scale PNs using multiple 3D image sets with different resolutions.

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References:

Poster / 130

On the grain drag in sands induced by polymer fluid flows

Author: Si Suo¹

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Polymer fluids, a blend of polymers in water, provide a cost-effective and environmentally sustainable solution for supporting deep underground excavations. Their support mechanism stems from the drag force exerted at the grain scale. However, as non-Newtonian fluids, their full potential in construction applications remains untapped due to limited understanding of their behavior. In this study, a specialized pore-network model (PNM) was developed to analyze polymer fluid flow in sands, alongside a custom module for calculating grain drag forces. This framework enables robust statistical analyses at the representative elementary volume (REV) scale. The model has been thoroughly validated through in-house experimental observations and detailed pore-scale numerical simulations. The insights gained from this work provide a scientific foundation for optimizing the design and risk management of deep excavation support systems utilizing polymer fluids.

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Large scale flow and dispersion in heterogeneous networks under non-linear flow conditions

Author: Marco Dentz¹

Co-authors: philippe gouze ²; Juan J. Hidalgo ¹; Jannes Kordilla ¹

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Large scale flow and dispersion in heterogeneous networks under non-linear flow conditions

Non-linear flow and dispersion in natural and engineered media are key issues in different fields of science and engineering. Applications range across scales from non-Newtonian flows in pore and capillary networks to turbulent flows in karst networks. Spatial variability in the physical medium properties lead to scale effects in the flow and dispersion processes that manifest in non-Fickian transport and non-Darcian flow behaviors. We study the mechanisms of flow and dispersion in two- and three-dimensional heterogeneous networks under turbulent and non-Newtonian flow conditions, that is, for flows in which the flow rate is a non-linear function of the pressure gradient. The flow fields are characterized statistically in terms of the distribution of Eulerian and Lagrangian flow velocities and their correlation properties with emphasis on the relation between network heterogeneity and flow statistics. Large scale flow is quantified by generalized (non-linear) Darcy and Darcy-Weisbach relations. Solute dispersion is measured in terms of particle breakthrough curves and displacement statistics. We observe broad distributions of particle arrival times and non-linear evolution of the displacement variance, which are manifestations of memory processes that occur due to broadly distributed flow velocities and mass transfer rates. These behaviors are linked to the medium structure and Eulerian flow statistics. Based on this analysis, we propose a stochastic time domain random walk approach to quantify the impact of the network heterogeneity on large-scale flow and dispersion.

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MS05 / 134

Impact of hydrodynamics on microbial transport and growth in porous-reservoir hydrogen storage

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Biofilms, aggregates of microbes encased in extracellular polymeric substances, are intricate systems where various chemical, biological, and physical processes occur, including attachment, growth, erosion, sloughing, and metabolite formation. Underground hydrogen storage (UHS) offers large-scale energy retention solutions using salt caverns, depleted hydrocarbon reservoirs, and saline aquifers. While biofilms can be beneficial in certain applications, such as leakage remediation, the food industry, and water quality management, they can pose challenges for UHS, particularly concerning hydrogen loss and injectivity. Numerical simulations can enhance our understanding of the interactions between biofilms and hydrogen during cyclic operations involving injection, storage, and withdrawal periods.

This contribution builds on the work presented at InterPore2024, titled “Field-scale Mathematical Modelling and Simulations of Biofilm Effects in Hydrogen Storage”. The previous study developed and implemented a mathematical model for field-scale UHS simulations, incorporating biofilm processes. Key mechanisms related to microbial activity include hydrogen consumption by the biofilm and porosity reduction due to biofilm growth. The fluid is modeled as a two-phase (liquid and gas), two-component (water and hydrogen) system, while the biofilm is modeled as a solid phase attached to the rock, growing through hydrogen consumption. The mathematical model was implemented in the industry-standard simulator Open Porous Media (OPM) Flow (Rasmussen et al., 2019). The existing hydrogen module was extended to include biofilms, providing flexibility to account for or neglect biofilm effects in simulations. Results of this implementation in OPM Flow were presented using the field-scale benchmark model from Hogeweg et al. (2022).

In this year’s contribution, the implementation of the mathematical model in OPM Flow is extended to include biofilm attachment and detachment. These additions introduce complex dynamics, particularly for hydrogen storage during injection, storage, and withdrawal intervals. We apply the model to assess hydrogen loss under various injection schedules and microbial parameters. The complexity of the geological models is increased from homogeneous radial reservoirs to heterogeneous field models, specifically SPE11C. For the homogeneous and heterogeneous radial reservoirs, we use the pyopmnearwell software (Landa-Marbán and von Schultendorff, 2023), an open-source framework for creating the necessary input files for OPM Flow (e.g., injection schedules, corner-point grids, tables for saturation functions) via configuration files, ensuring reproducibility of results and facilitating further studies (e.g., optimization, history matching). For the SPE11C study, we use the pyopmspe11 software (Landa-Marbán and Sandve, submitted), a Python framework using OPM Flow for the SPE11 benchmark project. Additional open-source tools related to OPM Flow can be found at <https://github.com/cssr-tools>.

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MS07 / 137

A Dynamic Network Model for Thermally-Driven Reactive Transport Near Chemical Equilibrium via Spectral Decomposition

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Predicting the fluid, thermal, and solutal transport in an evolving complex network of pores requires a fundamental description of the transport processes and their coupling to the underlying reaction chemistry. In a single pore, the complex dynamics under various competing timescales and solution-coupled boundary conditions give rise to nonmonotone behaviors in net fluid, thermal, and species fluxes across multiple parameter regimes: reactive (Damköhler), solutal-advective (Peclet) and thermal-conductive (Biot). To tackle a problem posed now in a pore network, we reduce the model order based on a small-amplitude perturbation analysis on the leading-order equations derived from an existing first-principle model [Tilley et al. 2021]. We characterize the dynamics on each edge (treated as a 1D interval) via a spectral decomposition of temperature and species transport near chemical equilibrium. We express the coupled pressure and pore radius evolution in terms of the spectral bases and forcings at adjacent vertices. By imposing flux conservation laws at network vertices via a weakly nonlinear analysis, we close the network model by describing the time evolution of temperature and species at interior vertices. This work introduces a general approach to pore network modeling with PDE dynamics near equilibrium and provides a firm analytical background for adaptation to nonlinear dynamics.

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MS06-A / 141

Simulation of Microcapsule Transport in Geothermal Reservoir Porous Matrices

Author: William Kibikas¹

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Geothermal energy is a critical application of subsurface utilization, offering a sustainable and renewable energy source. However, its widespread development faces significant challenges, particularly related to the high permeability of subsurface reservoirs. This characteristic often leads to non-ideal flow zones that hinder efficient heat extraction and reservoir performance. To address this issue, we are investigating using thermally degradable microcapsules to deliver high temperature nano-modified polymers to modify the permeability of larger, problematic fractures. For these materials to be effective, their transport behavior and tunable properties must be demonstrated experimentally and validated numerically before field-scale implementation.

We have developed a high-temperature high-pressure flow loop for injecting microcapsules into a porous network for 3 days at ~100 °C. We injected fluorescent polyethylene microcapsules into gravel matrices - simulating subsurface porous structures - while varying parameters during testing such as injection fluid viscosity, gravel size, and microcapsule properties. The results indicate that the microcapsule dimensions and densities allow for them to both flow into permeable zones and become trapped at certain points in the rock matrices. We observed that carrier fluid viscosity, microcapsule size, and gravel size all had effects on the quantity of microcapsules that became trapped in our samples versus flowing through the sample without trapping. We also used CT scanning to show that in most cases the microcapsules either completely passed through the gravel sample or sealed the near-entrance pore spaces. These tests complement ongoing tests using fractures to determine the relationship between the transport of microcapsules and fracture characteristics (aperture size, roughness, etc.). In addition, numerical models were developed to simulate how the physical properties of the microcapsules resulted in bridging and trapping and expand upon the microcapsule transport and trapping in alternate scenarios, such as fractured zones or more tortuous pore networks.

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References:

MS01 / 142

Dynamics of Ostwald ripening in underground hydrogen storage

Authors: Benzhong Zhao¹; Mohammad Salehpour¹

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Hydrogen is widely recognized as a promising solution for renewable energy storage, thanks to its versatility and high energy density. However, the challenge of seasonal hydrogen storage remains significant, with the absence of scalable storage solutions impeding the widespread adoption of green hydrogen. A 2022 report by the National Energy Technology Laboratory highlights underground hydrogen storage in deep saline aquifers and depleted gas reservoirs as the most viable options for addressing this need. In these systems, hydrogen is injected during periods of high renewable energy production and withdrawn during periods of low availability. This cyclic injection and withdrawal process leads to the formation of trapped hydrogen bubbles of varying sizes and shapes within the subsurface. These bubbles partially mix with the in-situ brine and undergo mass exchange via molecular diffusion, a phenomenon known as Ostwald ripening. The ripening process could have significant impact on the safety, injectivity, and purity of the storage operation.

Here, we study the dynamics of hydrogen bubble evolution in porous media through high-resolution microfluidic experiments. The microfluidic flow cell features a heterogeneous network of pores and throats, connected to boundary channels with larger apertures on the left and right sides. The disparate length scales generate chemical potential gradients that drive hydrogen diffusion from the porous matrix toward the boundary channels. The experiments were conducted at $T=40\text{ }^{\circ}\text{C}$ and $80\text{ }^{\circ}\text{C}$ and different initial gas saturations varying from $S=0.4$ to 0.6 . Each experiment lasted approximately two weeks, allowing sufficient time to capture the long-term dynamics of bubble evolution.

Our results reveal a distinct two-stage ripening process. The first stage involves a relatively slow equilibration phase, during which neighboring bubbles undergo ripening to minimize local variations in interfacial curvature. This is followed by a second stage, characterized by the diffusive loss of gas from the porous matrix to the boundary channels, exhibiting a characteristic diffusive scaling behavior. To further understand this phenomenon, we develop a continuum model of the ripening process that incorporates the capillary pressure-saturation relationship of the porous matrix. The model exhibits excellent agreement with experimental observations. These findings have significant implications for hydrogen storage operations, particularly in estimating equilibration timescales and assessing potential leakage rates in the presence of fracture conduits.

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MS03 / 143

Study of thermal protection system defects using a one-domain porous media model

Authors: Brandon Van Gogh¹; Bruno Dias²

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Humanity's innate drive for discovery has fueled exploration beyond Earth's boundaries, from landing on the Moon to ambitious missions targeting other planets and celestial bodies. Achieving these goals requires meticulous planning and engineering. Engineering uncertainty tolerances are gaining importance, mainly as mission objectives demand transporting larger payloads, such as life-sustaining equipment for Mars colonization. Spacecraft atmospheric entry poses large failure risk mitigation challenges due to extreme heat loads, with Thermal Protection Systems (TPS) playing a critical role in safeguarding missions. Ablative TPS materials, which degrade to protect spacecraft, can account for up to 50% of the total vehicle mass, impacting payload capacity. To address this challenge, NASA developed the lightweight Phenolic Impregnated Carbon Ablator (PICA) [1] in the 1990s. PICA has since been successfully utilized in missions like Stardust (2006), Mars Science Laboratory (2012) [2], and Mars 2020 [3].

The interactions between the aerothermal environment and the material result in highly coupled, multi-physics problems that are critical challenges in optimizing design margins and mission risk. These complex issues involve coupled multiple physical phenomena, such as heat transfer, material degradation, structural integrity, etc. posing critical challenges in optimizing design margins and mission risk. A significant challenge remains in understanding the material response in off-design scenarios when the TPS is subjected to unpredicted conditions not captured by ground experiments. These off-design scenarios include the possibility of TPS cavities on the shield that are generated by micrometeoroids and orbital debris (MMOD) impact [4]—an alarming issue due to the significant increase in space debris—or internal cracks propagation due to internal pressure build-up [5].

Enabling design by analysis requires the development of high-fidelity tools that couple flow and material behavior. A main challenge lies in developing suitable and robust numerical techniques that accurately track the material interface and in defining proper boundary conditions that capture material degradation [6]. The material response in the presence of defects introduces added complexities, such as augmented heating, pyrolysis gas flow driven by pressure gradients, alterations to heat conduction due to material anisotropy, etc. A main concern with MMOD impact while in transit include gas flow through porous cavity walls and potential mechanical material failure.

In this work, we study TPS defects using a one-domain porous media model [7] based on the volume-averaged Navier-Stokes (VANS) equations [8]. We generalize the governing equations to solve the flow field and the material in a unified approach [9]. The strong coupling between each phase mitigates modeling assumptions in conjugate heat-transfer coupling. This allows for a natural progression of the material interface due to heterogeneous reactions and the blowing of pyrolysis gases from the porous material without the need for complex boundary conditions.

During the lecture, we will show a series of TPS defect test cases under extreme spacecraft entry conditions utilizing the one-domain porous media model.

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Water & Porous Media Focused Abstracts:

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Poster / 144

Mineral precipitation shaped by flow, reaction and deposition kinetics

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Mineral precipitation and deposition during reactive flows through porous media are common phenomena in various natural and industrial processes, including biomineralization, marine sedimentation, water treatment, groundwater remediation, concrete carbonation, geothermal energy production, and geologic carbon sequestration. This process typically begins when fluids with different compositions mix and react, leading to supersaturation and the formation of solid-phase minerals. These solid precipitates can either remain suspended in the fluid, altering its apparent viscosity, or deposit onto the surfaces of the porous media, modifying the microstructure and influencing subsequent flow and transport behavior. While much of the literature on this problem has focused on the interaction between reaction and mixing, relatively few studies have explored the dynamics of suspension flow, and even less is known about how reaction and deposition interact with one another.

In this work, we propose a minimal ingredient model that can replicate qualitatively the myriad of complex flow patterns and quantitatively the macroscopic rate of precipitation as observed in past microfluidic experiments. The work highlights the need to capture both the rheology and deposition kinetics of the precipitate suspension in the continuum description of precipitation flow, even for systems with simple chemistry and infinitely fast reaction rates.

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MS05 / 145

Biogeochemical Reactions in Hydrogen Storage Salt Caverns: Sulfate Reduction in the Salado Formation

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Hydrogen storage in salt caverns offers a promising solution for large-scale energy storage; however, biogeochemical reactions involving hydrogen, minerals, and microbial communities can compromise hydrogen quality. The Salado Formation, a salt cavern located in west Texas and southeastern New Mexico, is composed of evaporites such as halite and interbedded potash salts like polyhalite, providing a unique geochemical environment for these interactions. This research focuses on sulfate reduction as the dominant microbial process in the Salado Formation, supported by ion analysis of core samples and Gibbs free energy calculations. Microbial activity in hydrogen storage caverns poses three key risks: i) economic losses due to hydrogen consumption and sulfate-induced corrosion, ii) health and safety hazards from hydrogen sulfide generation, and iii) increased purification requirements upon hydrogen withdrawal. To study these impacts, sulfate-reducing bacteria were isolated from coastal sediment near the Gulf of Mexico to ensure compatibility with the high-salinity brine of the Salado Formation. The bacteria were cultured in a brine solution modeled after Permian seawater in Salado Formation prior to evaporation, with sulfate serving as the electron acceptor and hydrogen as the electron donor during multiple cultivation cycles. Once a high population of sulfate-reducing bacteria was established, DNA extraction and 16S amplicon sequencing were performed to identify the microbial strains. The isolated sulfate-reducing bacteria were subsequently used in experiments to evaluate their effects on hydrogen storage. Experiments were conducted in sealed, anoxic serum bottles containing the modeled brine and isolated bacteria, under conditions representative of hydrogen storage salt caverns. Cores from the Salado Formation, including halite, polyhalite, and anhydrite, were introduced to the experiments to study their impact on brine salinity and sulfate content, simulating realistic cavern environments. Gas composition in headspace was monitored using Gas Chromatography, while sulfate reduction was quantified via Ion Chromatography. Hydrogen sulfide, a key byproduct of sulfate reduction contributing to gas contamination, was measured using Gas Chromatography and colorimetric methods involving reagents and a plate reader. By examining factors such as hydrogen pressure, salinity, and mineral concentrations, and the presence of formation cores, this study aims to quantify the extent of microbial-induced hydrogen loss and gas contamination. These findings provide critical insights into the biogeochemical challenges of hydrogen storage in salt caverns and strategies to mitigate these risks.

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MS23 / 146

Storage Criteria Evaluation for Underground Hydrogen Storage in Heterogeneous Aquifers

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Hydrogen has been recognized as a crucial energy carrier to reduce greenhouse gas emissions and facilitate the transition to a sustainable energy future. However, meeting the fluctuating energy demands solely through hydrogen production is not always feasible, necessitating the development of reliable storage solutions. Underground hydrogen storage (UHS) offers a promising approach to balance energy supply and consumption while ensuring energy security. Despite its potential, UHS is an emerging field of study with limited investigations, particularly on aquifer structural conditions that influence storage performance in heterogeneous aquifers.

In this study, underground hydrogen storage was numerically simulated in heterogeneous aquifers. First the important role of micro-scale heterogeneity on UHS performance was evaluated as micro-scale heterogeneity is often unaccounted for in reservoir-scale models. Then, aquifer thickness, dip angles and different boundary conditions were investigated as screening criteria for hydrogen injection and withdrawal during UHS in heterogeneous aquifers as different structural and boundary conditions can result in different UHS performance. Advancing research on these parameters will enable a more comprehensive understanding of storage dynamics and associated risks.

Results indicate that micro-scale heterogeneity significantly impacts hydrogen withdrawal during UHS. It creates a more complex flow regime and enhances localized hydrogen trapping in the aquifer. Variations in porosity and permeability at small distances exacerbate hydrogen immobilization, reducing overall recovery efficiency. This phenomenon underscores the critical need to incorporate detailed heterogeneity metrics in modeling and designing effective hydrogen storage systems, as neglecting these could lead to overestimations of storage capacity and recovery performance. Numerical simulation techniques can predict these effects, demonstrating the pronounced influence of micro-heterogeneities on hydrogen-brine displacement dynamics and residual gas trapping during operational cycles under different conditions including different thicknesses, dip angles and boundary conditions.

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Poster / 147

Fluid Inertia and Symmetry-Breaking Generate Global Chaotic Mixing in Laminar Porous Media Flows

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Solute mixing in porous media is a fundamental process that controls various industrial and environmental processes. Since pore-scale flows are typically steady and laminar, solute mixing was thought

to be largely driven by molecular diffusion. However, recent studies have shown that chaotic advection can emerge from 3D flow paths through the porosity [1, 2], strongly enhancing mixing as compared to 2D steady flow. In turn, we have observed that steady flows with weak inertia can also induce complex 3D flow structures in quasi-2D geometries, significantly enhancing local mixing [3-5]. The mechanism producing such enhancement is not yet fully understood.

In this study, we show that fluid inertia can induce global chaotic mixing in steady laminar flows through quasi-2D porous geometries. To do so, we use (1) Lagrangian particle tracking in direct numerical simulations of periodic geometries and (2) fluorescent solute imaging in microfluidic experiments. Numerical simulations were performed to study local fluid stretching rates and estimate Lyapunov exponents depending on the pore geometries. In turn, microfluidic experiments were performed to demonstrate the impact of Lagrangian chaos on scalar mixing rates, from creeping flow to inertial laminar flow regimes. Both periodic and random 2D porous geometries were investigated. Our findings reveal that in periodic porous media, fluid inertia induces localized chaotic mixing, resulting in local enhancement of mixing and transverse dispersion. Mixing remains limited by the persistence of mixing barriers, as evidenced by Poincaré maps. In contrast, flow symmetry breaking, characteristic of random porous media, leads to a dramatic increase in fluid mixing and transverse dispersion due to the emergence of global chaotic flow. This behavior is marked by the disappearance of mixing barriers, highlighting the roles of fluid inertia and symmetry-breaking in driving global chaotic mixing.

The insights gained have far-reaching implications for optimizing natural and engineered processes where fluid mixing is critical, such as contaminant transport and carbon mineralization in fractured media, and biochemical reactions in micromixers.

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MS06-B / 148

Phase-field modeling of snow microstructure evolution

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The microstructure of snow determines its fundamental properties such as the mechanical strength, reflectivity, or the thermo-hydraulic properties. Snow undergoes continuous microstructural changes due to local gradients in temperature, humidity or curvature, in a process known as snow metamorphism. Dry snow metamorphism occurs at temperature below the melting point where the snow is assumed to be absent with liquid water; wet snow metamorphism occurs when temperature is close to the melting point and involves phase transitions amongst liquid water, water vapor, and solid ice. In this work, we describe our recent efforts in developing a pore-scale phase-field model that simultaneously captures the three phase-change phenomena relevant to snow metamorphism: sublimation (deposition), evaporation (condensation), and melting (solidification). The phase-field formulation allows one to track the temperature evolution amongst the three phases and the water vapor concentration in the air. Our three-phase model recovers the corresponding two-phase transition model when one phase is not present in the system. We perform 3D simulations of the two-phase model to study sintering of ice particles (i.e., dry metamorphism) and find that the model can reproduce the neck growth rate measured in controlled laboratory experiments at two different temperatures. We then perform 2D simulations of the three-phase model to study the impact of humidity and temperature on the dynamics of wet snow metamorphism at the pore scale. We explore the role of liquid melt content in controlling the dynamics of snow metamorphism in contrast to the dry regime, before percolation onsets. The model can be readily extended to incorporate two-phase flow and may be the basis for investigating other problems involving water phase transitions in a vapor-solid-liquid system such as airplane icing or thermal spray coating.

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Poster / 149

Effects of fluid density and inertia on solute transport at fracture intersections: Visual laboratory experiments and pore-scale numerical simulations

Author: Porraket Dechdacho¹

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Flow and transport in fractured media are governed by complex interactions between geological heterogeneity and fluid properties. In subsurface systems, fluids with different densities often coexist, leading to density-driven flow that can impact flow and transport. Additionally, in fractured systems where high flow velocities are common, fluid inertia can further influence transport dynamics by inducing vortices, creating mixing hotspots, and enhancing reaction rates at fracture intersections. Understanding the interplay between these processes is crucial for subsurface applications, including saltwater intrusion, enhanced geothermal systems, and geologic carbon sequestration. While previous studies have explored either density-driven flow or inertia effects on solute transport, the combined influence of these factors on solute transport in fracture networks remains poorly understood. This study combined pore- to network-scale visualization experiments and numerical simu-

lations to investigate how fluid density contrast coupled with fluid inertia governs solute transport and retention in fractured media.

At the network scale, artificial fracture networks were constructed from transparent acrylic blocks to enable 3D visualization of transport processes. A fluorescent dye, with a density 21% denser than the ambient water, was injected as a tracer. We observed persistent vortices emerging at vertical fractures near fracture intersections, leading to localized solute trapping within the network. To further examine the underlying mechanisms of this trapping behavior, we developed a bench-top-scale visualization apparatus focused on a single fracture intersection. This apparatus, constructed from clear acrylic sheets, features two smooth horizontal fractures connected by a vertical fracture, with a constant aperture of 0.5 cm. A series of controlled experiments were conducted to investigate the roles of density contrast, fluid inertia, and flow imbalance on solute trapping. Image analysis was performed to quantify tracer concentration evolution within the vertical fracture and breakthrough curves in the horizontal fractures.

The experimental results demonstrated that the combination of density contrast and inertia effects leads to enhanced solute trapping. The density contrast allows the dye to sink into the vertical fracture, and vortices induced by fluid inertia trap the tracer within the vertical fracture, significantly enhancing solute retention. The localized vortices emerge at the base of the vertical fracture, trapping the dense tracer in recirculation zones over an extended period. Maximum solute trapping was observed when the flow rate in the bottom horizontal fracture was 10% higher than that in the top horizontal fracture, effectively balancing the downward flow of the denser fluid. This emphasizes the critical interplay between density effects and inertia effects, which significantly control solute retention at fracture intersections. Pore-scale numerical simulations reproduced the localized trapping observed in experiments and revealed detailed insights into the key processes governing solute transport, including the emergence of recirculation zones, the dynamics of vortices affected by density effects, and the influence of flow imbalance on velocity field leading to maximum solute retention. Our results highlight the importance of small-scale processes, such as vortex-induced trapping of dense fluids, in controlling flow and transport dynamics at larger scales. These insights provide valuable fundamental understanding relevant to various subsurface engineering applications.

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Pore-Scale Investigation of a Novel Method for the Remediation of Soils Polluted by Chlorinated Solvents Based on Compositional Ripening Using Pickering Emulsions

Authors: Antonio Rodríguez de Castro¹; Azita Ahmadi²; Aziz OMARI³; Fernando LEAL-CALDERON⁴; Shuxin WANG⁵

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Chlorinated organic compounds (COCs) exhibit instability, toxicity, volatility, and limited solubility in groundwater, all of which can lead to secondary contamination [1, 2]. Zero-valent iron (ZVI) particles were first considered in the late 1970s for COCs remediation [3]. The increase in the reactivity of nano zero-valent iron particles (nZVIs) was mainly attributed to the increase in the specific surface area, which provide a greater number of active sites on which reactions occur. However, nZVIs face limitations, including rapid oxidation by air and water, and a tendency to aggregate and sediment. This results in a rapid decrease in their specific surface area, reactivity, and mobility [4]. To protect nZVIs from rapid corrosion and enhance their transport in aquifers, we introduce Pickering emulsions to encapsulate nZVIs and facilitate their transport through porous media. Additionally, Pickering emulsions have proven effective for physical in situ remediation [5]. This study aims to investigate emulsion flow dynamics, fluid phase distribution within pores, and the mechanisms of TCE removal through well-controlled pore-scale experiments in microfluidic chips.

The microchip used was water-wet, with a pore-width distribution ranging from 4 to 440 μm (Figure 1a) and a constant depth of 20 μm . Its porosity and absolute permeability were 0.52 and 2.5 Darcy, respectively. The Pickering emulsions were formulated using rapeseed oil with nZVIs (0.2 wt%) and silica nanoparticles (2.5 wt%) as stabilizers. To render the silica nanoparticles partially hydrophobic, tetradecyltrimethylammonium bromide (TTAB, 0.027 wt%) was added to the continuous phase, while oleic acid (0.2 wt%) was added to the dispersed phase to prevent large-scale aggregation of nZVIs. The TCE was dyed for clear visualization in the microchip, then brought to residual oil saturation (Sor) after a Pickering emulsion flooding step. The experimental setup consisted of three main components: the fluid injection, the optical, and the microfluidic control systems. A schematic diagram of the setup is shown in Figure 1b. Variation in Sor over aging time at a static state was observed under a microscope, with acquired images segmented and processed using ImageJ software.

Our results first showed that the Pickering emulsion droplet diameters were significantly smaller than the pore widths (Figure 1a), which helped prevent substantial emulsion droplet break-up during transport. Emulsion flooding enabled physical displacement, achieving an Sor of 10%. Flow was stopped after emulsion injection. After 15 hours of aging under static conditions, the size of the emulsion droplets significantly increased due to ripening (Figure 2), while the trapped TCE gradually decreased. This process is driven by compositional ripening, during which TCE transfers through the emulsion's continuous phase into the droplets. This transfer promotes good contact between TCE and nZVIs, which is expected to facilitate the initiation of TCE reduction. Ongoing experiments using gas chromatography for the analysis of the effluents will allow to confirm TCE degradation.

In conclusion, Pickering emulsions encapsulating nZVIs show promising potential for effective TCE degradation. Beyond effective physical displacement, this approach enables TCE mass transfer into droplets. This study proposes an innovative and environmentally friendly technology for in-situ degradation of soil pollutants.

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MS13 / 152

Micro-occurrence of gas and water in shale nanopores

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The micro-occurrence of gas and water in shale nanopores under reservoir conditions, as well as the changes in their distribution following the infiltration of fracturing fluids, are critical for understanding the behavior and flow dynamics of gas and water during shale gas extraction. Small-angle and ultra-small-angle neutron scattering (SANS/USANS) experiments conducted under high-pressure and vacuum conditions have elucidated the occurrence state of methane within shale nanopores. Additionally, dynamic water vapor sorption measurements at varying temperatures have documented changes in water distribution within these nanopores.

To further investigate the process of fracturing fluid penetration into nanopores, a combination of field emission scanning electron microscopy (FE-SEM) and cryogenic scanning electron microscopy (cryo-SEM) was employed. These observations were performed following Wood's metal impregnation and spontaneous imbibition with deionized water. Furthermore, SANS/USANS experiments conducted under high-pressure conditions with coexisting gas and water revealed changes in micro-occurrence state of methane after fracturing fluid penetration.

SANS/USANS data collected under ambient and high-pressure conditions quantified the fraction of pores accessible to methane. The confinement effects observed indicated that the density of methane in pore spaces smaller than 20 nm under high pressure exceeded that of an ideal gas at the same pressure. This density further increased as pore sizes decreased, forming nanoscale methane clusters with densities several times higher than their inert state. Dynamic water vapor adsorption experiments demonstrated that as temperature increased, the affinity of monolayer water molecules to the shale surface diminished, reducing the formation of chemical bonds. Concurrently, the adsorption force between multilayer water vapor molecules decreased, with the maximum adsorption capacity primarily influenced by the nanopore structure.

FE-SEM observations revealed that molten Wood's metal penetrated the shale matrix from microfractures under high pressure. The extent of Wood's metal infiltration into matrix pores served as an indicator of the degree of microfracture development in the shale and the connectivity between matrix pores and microfractures. Cryo-SEM observations further demonstrated that fracturing fluid (water) infiltrated microfractures in a stratified manner due to spontaneous imbibition. Simultaneously, the fluid entered matrix nanopores in the form of water films or water bridges. Within organic matter nanopores, the fracturing fluid predominantly appeared as water films.

Based on SANS/USANS analysis, it was observed that when methane and water coexist in shale nanopores, the pores were predominantly occupied by water, which exhibits a stronger adsorption affinity than methane. Consequently, methane desorbs from the matrix pores and migrates into microfractures. This finding suggests that during hydraulic fracturing of shale gas reservoirs, a

lower flowback rate of fracturing fluid is favorable for achieving higher gas production. Prolonging the borehole closure time facilitates displacement efficiency of gas and liquid within shale nanopores, thereby enhancing methane recovery rates.

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Coupled THM Processes in PFLOTRAN for Modeling Enhanced Geothermal Systems

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Numerical modeling of coupled thermal, hydraulic, and mechanical (THM) processes is crucial for understanding and capturing the complex interactions in enhanced geothermal systems (EGS). We describe the development of the numerical approach for coupling those processes to improving the predictive capabilities for the EGS testbed site, part of the Center for Understanding Subsurface Signals and Permeability (CUSSP). In PFLOTRAN, fluid flow and heat transport are modeled using TH mode which is sequentially coupled with a linear elasticity model for capturing the geomechanical stress response by deformation of the subsurface. Biot's model and the coefficient of thermal expansion are integrated to capture fluid flow and thermal effects, respectively, in geomechanics. The geomechanical solution contribute to changing the rock properties such as porosity and permeability. The pressure and temperature constitute the primary unknowns when solving the fully coupled system of the mass and the energy conservation equations in TH mode employing the finite volume approach. The displacement is the primary unknown in the quasi-static geomechanical problem and solved with the finite element approach. We aim to present how the geomechanics process model is integrated into PFLOTRAN frameworks and describe the sequential solution strategy for solving the thermo-poro-elasticity problems. We demonstrate the advancement of PFLOTRAN process model coupling for THM processes with numerical experiments for enhanced geothermal systems.

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MS08 / 154

Dispersed two-phase flow for mixing enhancement in porous media**Author:** Yang Liu^{None}**Co-author:** Moran Wang¹¹ Tsinghua University**Corresponding Authors:** mrwang@tsinghua.edu.cn, liuyang20@mails.tsinghua.edu.cn

Efficient solute mixing in porous media is crucial for various natural processes and industrial applications, such as nutrient transport in biological systems, groundwater bioremediation, carbon dioxide-enhanced oil recovery, and packed-bed reactors. The effectiveness of solute mixing directly influences the rates of biological and chemical reactions in these scenarios. While turbulence is commonly used to enhance mixing due to its transient and chaotic flow dynamics, its effectiveness in porous media is constrained by the extensive solid boundaries that suppress turbulence. Alternatively, dispersed two-phase flows, which feature transient flow behavior [1] and are more feasible to porous media, offer a promising strategy for improving mixing efficiency.

The current understanding of solute mixing driven by dispersed two-phase flow remains incomplete. Research on enhancing mixing through these flows has largely concentrated on simple systems [2], such as uniform channels or bulk fluids, without considering the complexities of porous media. On the other hand, most investigations into solute transport within porous media under two-phase flow conditions assume static phase interfaces [3]. However, dispersed two-phase flows are inherently characterized by dynamic and evolving phase interfaces. This gap in knowledge regarding the performance and mechanisms of dispersed two-phase flow on solute mixing within porous media hinders a comprehensive understanding and modulation of its behavior.

This study investigates transverse mixing driven by dispersed two-phase flow in porous media using pore-scale direct numerical simulation. Results indicate that dispersed two-phase flow exhibits transient features, such as the formation of vortices, which are absent in single-phase flow. These transient characteristics, particularly the vortex structures, significantly enhance transverse solute mixing. The efficiency of mixing is evaluated using the mixing volume ratio, defined as the proportion of the volume where solute concentrations range between 0.01 and 0.99 relative to the total solvent volume. At identical total injection flow rates, the mixing volume ratio for dispersed two-phase flow is approximately twice that of single-phase flow. These findings offer novel insights for enhancing mixing in porous media.

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MS06-A / 155

Experimental study on spontaneous imbibition characteristics of tight glutenite reservoirs

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Spontaneous imbibition plays a critical role in two-phase flow within hydraulic fractures of tight reservoirs. Despite significant efforts to address this phenomenon, there are few studies that concentrate on tight glutenite reservoirs, an essential subset of tight reservoirs. As a result, the imbibition mechanism and its influencing factors remain unclear, with several key factors not being captured, and in-depth analyses missing in spontaneous imbibition for tight glutenite reservoirs. Given the existing knowledge gaps, this study performed a series of water imbibition experiments in conjunction with X-ray diffraction, thin section analysis, scanning electron microscope observations, and high-pressure mercury injection tests on tight glutenite cores exhibiting various petrophysical properties. The influences of mineral composition and content, concentration of particles with different sizes, pore type and structure on spontaneous imbibition were revealed. The main and secondary influencing factors were identified through grey relation analysis. The experimental results indicate that distinct microscopic characteristics of tight glutenites lead to significant variations in spontaneous imbibition patterns. Consequently, the experimental cores were categorized into two groups. For Group I, intergranular pores filled with water-wet quartz grains and illite, as well as gravel-edge fractures connected with pores, can significantly enhance imbibition recovery. Intragranular dissolved pores and medium-size sand are negative influencing factors. However, in Group II, intergranular pores and gravel-edge fractures are filled with oil-wet chlorites and matrix, respectively, which hinders water imbibition. The interconnected intragranular dissolved pores are the primary spaces for water imbibition. Micro and macropores can enhance water imbibition and oil drainage ability, respectively. Thus, their coordination facilitates spontaneous imbibition. Macropores and gravels are the primary influencing factors for Group I, whereas for Group II, the main influencing factors include medium-sized sand, intragranular dissolved pores, fractal dimensions, micropores, and intergranular pores. These observations enhance our comprehension of the unique imbibition mechanisms present in tight glutenite reservoirs.

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MS19 / 156

Impact of Diffusion Media on Performance and Durability in Electrochemical Systems

Author: Siddharth Komini Babu¹

Co-authors: Jacob Spendelow¹; Rod Borup¹; Sergio Diaz Abad¹; Tanvir Arman¹; Yuanchao Li¹

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Diffusion media are an integral component in electrochemical systems including fuel cells, water electrolyzers, and unitized reversible fuel cells (URFCs). Diffusion media facilitates efficient transport of reactants and products to and from the catalyst layer, enabling electron conduction, and providing mechanical support and thermal management. Advancing our understanding of the key properties of diffusion media—including pore size distribution, porosity, and wettability—is crucial for enhanced two-phase mass transport. By optimizing these functions, diffusion media directly influence the overall performance, efficiency, and durability of these systems enabling next-generation energy technologies. In this presentation, we will delve into the specific properties of diffusion media that impact both performance and durability, emphasizing their pivotal role in advancing electrochemical energy systems.

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References:

157

Robust wettability manipulation via nanoparticle adsorption with implications for multiphase flow control in disordered media

Author: Xukang Lu¹

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Wettability manipulation is crucial for controlling multiphase flow in porous media and diverse other practical applications. Here, we introduce spontaneous nanoparticle adsorption from suspensions onto solid surfaces as a convenient yet effective way to tune surface wettability. Combining experimental characterizations and theoretical modeling, we present a comprehensive description of variable particle size effects on microscopic adsorption kinetics and macroscopic modification performances under varying salinity and surface charging conditions. We evidence that robust modification can be achieved by aligning particle properties with environmental conditions, and identify an intermediate size range consistently benefits wettability variation. Extending static analysis, we systematically explore how intrinsic wettability and structure heterogeneity influence nanoparticle-assisted multiphase displacement in complex porous geometries by microfluidic experiments, revealing distinct dynamic patterns governed by the above factors. Our work sheds light on the application

of nanoparticle suspensions for surface property and flow control in geological systems and engineering porous media.

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MS20 / 158

Measurement of permeability coefficient of biological very soft matter

Authors: Soonmoon Jung^{None}; Jaemin Kim¹; Junghwa Hong²

Co-authors: Youngho Lee¹; Hyeyeong Song¹; Jiwoo Jang¹; Seungyun Oh¹; Inyeop Na¹

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The human skeletal sponge bone is composed of hard porous materials (pore diameters of 100 to 500 μm) filled with the red marrow (BM). BM provides microenvironments for bone remodeling and hematopoietic function. BM cells form the marrow extracellular space, which is filled with intramarrow fluid (IF) and is flexible enough to allow migration, deformation, interaction, and metabolism of the BM cells. For the interaction and metabolism of BM cells, intramarrow fluid flow (IFF) must occur in the BM. The IFF is caused by pressure of sinusoids (1.78 to 2.73 kPa), which regulate intramarrow fluid pressure gradients (IFP).

The IFF is governed by permeability of the BM (κ) and the IFP. Changes in κ could affect changes in the BM extracellular space and IFF (IFF shear stress and BM cell migration). Therefore, changes in κ could result in changes in structural interaction, metabolism, hematopoiesis, and osteogenesis of the BM cells. However, κ is never measured since the BM has an extremely soft matter and is fragile in vitro.

An apparatus was applied to 16 bovine vertebral trabecular cylinders 10 mm in diameter and length to induce the caudal-cephalic IFF during compressive loading (0.3% strain). A pressure transducer was placed at the bottom of the samples to monitor IFP. Two electrodes were inserted at the bottom and top of each sample to measure the streaming potential gradient (SPG).

The measured IFP and SPG were $2500 \pm 268 \text{ Pa}/0.01\text{m}$ and $11.85 \pm 3.21 \text{ mV}/0.01\text{m}$. The permeability was $3.82 \times 10^{-12} \pm 2.44 \times 10^{-11} \text{ m}^2/\text{Pa}\cdot\text{s}$ based on the poro-electrokinetic: $\kappa = \sigma_0 \left(\frac{\nabla v}{\nabla p}\right)^2$ where σ_0 is BM electric conductivity of 0.17 [S/m] [Balmer, et.al, 2018], ∇v is SPG [V/m], and ∇p is IFP [Pa/m].

The value of κ could depend on the stiffness, shape, and distribution of the BM cells as well as the ECM. For example, a higher proportion and clustering of adipocytes significantly reduces κ , which significantly reduces the IFF. A pathological remodeling of the ECM such as myelofibrosis could lower the value of κ , which results in changes in the fluid-to-porous solid properties of the BM. As a result, changes in κ could cause changes in the metabolism, differentiation, proliferation, and migration of BM cells as well as the metabolism and bone remodel signaling of the osteocytes in trabeculae. It could be suggested that measuring changes in κ using MRI [Daldrup-Link, et.al, 2000] may be used

as a noninvasive early detection tool for diagnosing pathologies related to hematopoiesis and osteogenesis.

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Experimental Study on the Recovery of Immature and Low-Maturity Shale Oil Using In-Situ Combustion

Authors: Hong Zhang¹; Fajun Zhao¹

Co-authors: Xiaolin Wu²; Xin Liu²; Yu Qian³; Jiawei Li⁴

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² *State Key Laboratory of Continental Shale Oil*

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The Gulong shale oil resources in the Songliao Basin are abundant, predominantly concentrated in the Qingshankou and Nenjiang Formations. Immature to low-maturity shale is widely distributed, particularly in the first and second members, with a maturity level (Ro) generally below 0.75%. In-situ transformation methods can convert the organic matter within immature and low-maturity shale into recoverable oil and gas. Among these methods, in-situ combustion heating is a promising technique, though it is still in the early stages of development. This study presents laboratory experiments on in-situ combustion heating for immature and low-maturity shale oil. The optimal combustion temperature range was identified as 400–450 °C based on an analysis of heavy-component combustion products. The experiments showed that organic carbon combustion in shale oil from the Daqing area releases heat, consuming 2.25% of the total mass at 450 °C. With an organic carbon energy release of approximately 40 MJ/kg (comparable to conventional crude oil at 41 MJ/kg) and a reference recovery rate of 65% under field conditions using red-light fire flooding, it was estimated that 20% of the dissipated heat could transfer to the top and bottom cover layers. Moreover, 1 m³ of shale oil can achieve a temperature of 478.77 °C using its self-generated energy, which is equivalent to injecting 702.6 tons of 400 °C steam into the reservoir. This process facilitates steam heating, in-situ upgrading of immature and low-maturity shale oil, and supports green electric heating initiatives. This study underscores the potential of in-situ combustion heating as a viable and efficient technique for the recovery of immature and low-maturity shale oil. It provides a theoretical basis for advancing the green, low-carbon, and efficient development of these resources.

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160

Challenges in modeling water filtration by adsorbing porous media using Volume Averaging Method

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Volume Averaging Method (VAM) is a respected mathematical technique to upscale from pore to lab scales which has been used in diverse areas including water filtration, wicking, composites manufacturing, and groundwater flow. In porous water filters, the transport and entrapment of contaminants can be modeled as the classic mass transport problem, which employs the conventional convection-dispersion equation to predict the contaminant concentration. Upscaling using VAM has revealed two possible macroscopic equations for predicting contaminant concentrations in the filters. The first equation is the classical convection-dispersion equation, which incorporates a total dispersion tensor. The second equation involves an additional transport coefficient, identified as the adsorption-induced vector. In this study, the aforementioned equations were solved in 1D for column tests using 3D unit cells. The simulated breakthrough curves (BTC), using the proposed micro-macro coupling based VAM, are compared with the direct numerical simulation (DNS) results based on BCC type unit cells concatenated in daisy chain manner, as well as with three previously reported experimental works, in which the functionalized zeolite and zero valent iron fillings were used as adsorbent to remove phosphorous and arsenic from water, respectively. The disagreement of VAM BTC predictions with DNS and experimental results reveals the need for an alternative closure formulation in VAM. Detailed investigations point to time constraint violations in all three cases, suggesting this as the main cause of VAM's failure.

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161

Effect of Cyclic Hysteresis on the Storage Efficiency and Recovery of Underground Hydrogen Storage in a US Gulf Coast Saline Aquifer

Author: Mohamed Abdelaal¹

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Abstract

The accelerated consumption of fossil fuels has led to an unprecedented increase in the anthropogenic carbon emissions to the atmosphere. In the recent few decades, several efforts have been devoted to expand the use of renewables as alternative energy resources. Nevertheless, the intermittent nature of renewable energy causes fluctuations in energy supply, positioning hydrogen (H₂) as a promising and reliable energy carrier for peak demand. Geological porous media represent promising underground hydrogen storage (UHS) sites given their high storage capacity, global availability, and reduced microbial activity in saline conditions. However, the cyclic nature of UHS in geological saline formations introduces significant hysteresis effects on the relative permeability of hydrogen and brine. This impacts the hydrogen storage capacity and recoverability. Specifically, hysteresis reduces the non-wetting phase's mobility and enhances residual hydrogen trapping. This increases the critical hydrogen saturation required to initiate flow after each injection-withdrawal cycle, leading to diminished storage efficiency and recovery rates. Nevertheless, the impact of the relative permeability hysteresis on hydrogen-brine flow behavior, and its implications for storage capacity and recovery, remain underexplored. Most UHS studies rely on non-hysteretic models which neglect the cyclic drainage and imbibition processes inherent to the hydrogen injection-withdrawal process. This gap is also critical, as hysteresis-induced effects such as plume stabilization, brine upconing, and reduced withdrawal efficiency directly influence the feasibility of UHS. Additionally, in contrast to CO₂ storage, residual trapping has a significant impact more than dissolution trapping given the hydrogen's low solubility in brine. This underscores the need for a detailed analysis of hysteresis in hydrogen storage systems. Several studies have been devoted in the literature to address the hysteretic effect for CO₂ storage in saline aquifers, but not for H₂ storage, which is the goal of this study.

Methodology

We model hydrogen storage in a saline formation to address this research gap. The aquifer and fluid properties are representative of a potential UHS site in the US Gulf Coast region. We utilize CMG-WinProp to predict the phase behavior of the hydrogen-brine system, and CMG-GEM for the dynamic reservoir simulations. WinProp enables accurate estimation of the thermodynamic properties across a wide range of practical reservoir conditions. This includes phase equilibria, H₂ dissolution in brine, interfacial tensions, and capillary pressures. GEM facilitates a comprehensive evaluation of cyclic hydrogen injection-withdrawal processes, integrating hysteretic relative permeability models to capture the cyclic effects of drainage and imbibition. Experimentally derived hysteresis models – obtained from the literature – are employed to assess their influence on the dynamics of storage. This includes hydrogen saturation distribution, residual trapping, and withdrawal efficiency. The study also explores operational strategies such as injection rates and shut-in periods to optimize storage performance and mitigate relevant challenges. Numerical sensitivity analyses are conducted to further quantify the impacts of varying geological and operational parameters on recovery factors and storage efficiency. The findings aim to inform importance of the hysteretic nature of UHS in saline aquifers which provides critical insights into optimizing simulations for hydrogen storage in saline reservoirs under cyclic conditions.

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Effects of SO₂ on CO₂ mineral sequestration in different basalt minerals**Authors:** Zhe Wang¹; Lifu Zhang¹¹ College of Marine Science and Technology, China University of Geosciences (Wuhan)**Corresponding Authors:** wangzhe549@outlook.com, zhang-lifu@cug.edu.cn

Co-injection of CO₂ with water can be used to achieve rapid and efficient storage of CO₂ in minerals. In order to reduce the injection cost, the co-injection of CO₂ containing acidic impurity gas with water can effectively improve the feasibility of storage. However, the acidic impurity gas is more acidic than CO₂ and will react earlier than CO₂. This could inhibit the mineral sequestration process. Therefore, it is necessary to study the specific effects of co-injection of CO₂ containing acidic impurity gas and water on mineral storage in basalt reservoir. Considering the complexity of mineral types in basalt, we select olivine, diopside and anorthite to carry out experiments to compare the reaction difference of different minerals. We used transparent silica capillary tube to investigate the reaction process of CO₂-SO₂-water and minerals under geological reservoir conditions. In situ Raman spectroscopy is used to quantitatively observe the change process of the composition of the solution and minerals, and reveal the influence of SO₂ on the carbonation reaction of different minerals. The results show:

1. The presence of SO₂ will accelerate the dissolution process of basalt minerals, and SO₂ will react quickly after injection. In particular, in the reaction with anorthite, SO₂ is completely consumed within an hour, while CO₂ takes several days to react with the mineral.
2. The cation of olivine is Mg²⁺, which cannot react with SO₂ to form precipitation. At this time, the main effect of SO₂ is to reduce the pH of the solution, accelerate the dissolution of olivine, and promote the process of mineral carbonation.
3. Both anorthite and diopside contain Ca²⁺, so they react with SO₂ to form minerals such as calcium sulfite. The mineral will show the needle morphology, especially near the interface of the gas.
4. Although SO₂ reacts very quickly with minerals near the interface, it will still react with minerals far away from the gas, but the reaction is weak.

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163

Gas mixing driven by temperature gradient between H₂ and CO₂ cushion gas: implication for underground hydrogen storage**Authors:** Zhe Wang¹; Lifu Zhang¹; Wanjun Lu¹; Huirong Guo²; Yuhang Wang²

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² School of Environmental Studies, China University of Geosciences (Wuhan)

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Underground hydrogen storage (UHS) is considered feasible for storing large amounts of hydrogen (H₂). The injection and extraction of H₂ will result in significant temperature differences between the wellbore and reservoir. The thermal diffusion driven by the temperature gradient (Soret effect) may enhance the mixing between H₂ and cushion gas, which could decrease the purity of the produced H₂. Unfortunately, limitations of existing experimental methods have led to limited quantitative studies of thermal diffusion between H₂ and cushion gases under reservoir conditions. In this work, the thermal diffusion process of H₂ and CO₂ under reservoir conditions is quantitatively observed for the first time. Results show that the Soret effect drives H₂ accumulation in the high-temperature region, and is influenced by temperature, pressure, and concentration. There is significant concentration difference between the high- and low-temperature sections when minor quantities of gas are injected. From experimental observations, the Soret coefficients are obtained across different physical conditions and a correlation for their prediction is proposed. Additionally, while thermal diffusion slows down in porous reservoirs, the concentration difference established along the temperature gradient remains unchanged at steady state.

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164

A dynamic network model for forced imbibition considering local interplay of capillary and viscous forces

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¹ KTH Royal Institute of Technology

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The pore-scale interfacial dynamics including main-meniscus flow and corner flow usually occurs in heterogeneous porous media and significantly affects the macroscopic multiphase flow process. The numerical research on the competition between main-meniscus flow and corner flow remains challenging, particularly its upscaling in porous media due to the large spatial and temporal scale difference. We proposed a critical capillary number (Ca) by considering the interplay of local capillary and viscous forces, which predicts transition from main-meniscus flow into corner flow during the strong imbibition. The critical Ca model was employed to establish a dynamic network model by upscaling the pore-scale interfacial dynamics with the multiphase flow in porous media. The forced imbibition in heterogeneous porous media with various depths under different Ca were simulated and compared to microfluidic experimental data. The comparison indicates that the dynamic competition between main-meniscus flow and corner flow vitally affects the displacement behaviors predicted by pore-scale modelling, and our dynamic network model accurately captures the interfacial dynamics

observed in the microfluidic experiments. Moreover, the impact of interfacial dynamics on macroscopic multiphase flow pattern and displacement efficiency in heterogeneous porous media were addressed during strong imbibition under various viscosity ratios and capillary numbers. The phase diagram manifests a monotonic effect of viscosity ratio on displacement efficiency at high Ca due to the dominance of viscous fingering. A non-monotonic effect of viscosity ratio is revealed at low Ca, which is ascribed into competition between corner flow and main-meniscus flow.

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References:

MS15 / 167

Advanced Pore Network Modelling (PNM) for Packed-Bed Reactors: A Neural Network Approach Using PR-CFD Data

Author: Cristina García Llamas¹

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Packed-bed reactors are widely used due to their efficient heat and mass exchange. The hydrodynamics of these reactors is largely influenced by particle-fluid interactions. However, a unified theory representing the effect of particle shape on flow distribution and global parameters such as pressure drop is not well-described in the literature. Studying the hydrodynamics in a packed bed using Particle Resolved Computational Fluid Dynamics (PR-CFD) techniques represents an excellent alternative to experimentation. Nonetheless, PR-CFD is computationally expensive, whereas less resolved methods like Pore Network Modeling (PNM) offer a viable alternative. The accuracy of PNM simulations depends largely on the definition of physically accurate calibration factors, which can be derived from highly resolved PR-CFD simulations. This research aims to train an Artificial Neural Network (ANN) using PR-CFD data to obtain physically accurate calibration coefficients for various particle packings and particle size distributions.

We focus on packed bed reactors where the spacing between the walls is sufficiently large to disregard the influence of confining walls. We adopt a unit-cell approach, where the packed bed configuration is derived by periodically repeating this unit-cell in all three dimensions. This method has proven effective in modeling transport processes under steady-state conditions.

- Particle Resolved Computational fluid Dynamics (PR-CFD)
The Navier-Stokes and continuity equations are solved under the assumption of incompressibility conditions. The computational domain is discretized with a conformal mesh composed of hexahedral elements. Periodic boundary conditions are applied across all domain boundaries.
- Pore Network Modelling (PNM)
The PNM model utilizes the 3D structure information of the packed bed to generate a network of pores and throats. The hydrodynamic equations are solved by computing the mechanical energy and mass balance equations for each pore-throat-pore element. The overall pressure drop is model

using a variation of the Hagen-Poiseuille equation that accounts for frictional losses. Due to the simplification of the particle packing into a pore network, the frictional forces associated with the particle shape are not properly described. Therefore, a resistance term should be incorporated to account for the local pore geometry. To obtain this resistance term, a calibration procedure is performed using an Artificial Neural Network (ANN), which is explained below.

- Calibration of the PNM model using an Artificial Neural Network (ANN)
PR-CFD simulations are conducted using a wide range of particle packings. The ANN is trained using this particle-resolved Computational Fluid Dynamics (CFD) data, where each throat within a pore network serves as an individual data point for model training. The flow resistances associated to each throat are determined across a broad spectrum of local pore geometries. These flow resistances can subsequently be integrated into the PNM model as inputs to accommodate the throat-specific flow resistance associated with the local geometry.

This methodology enables physically accurate PNM simulations of packed beds for a wide range of particle shapes and polydispersities at a relatively low computational cost, which is critical for an optimal design of packed bed reactors.

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Poster / 168

Effects of Pore-Scale Three-Dimensional Flow and Fluid Inertia on Mineral Dissolution

Authors: Woonghee Lee¹; Michael Chen¹; Etienne Bresciani²; Brandy Toner¹; Peter Kang¹

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Mineral dissolution is a key process of subsurface systems and engineering applications, such as karst formation and engineered carbon mineralization. Fluid flows have been shown to significantly affect mineral dissolution rates by controlling concentration fields [1-2], highlighting the importance of understanding flow-dissolution dynamics. In subsurface porous and fractured media, inertial flows can readily occur and induce complex flow structures, such as recirculating flows, which complicate mineral dissolution dynamics. Moreover, recent studies demonstrated that flow topologies can fundamentally differ between 2D and 3D systems, particularly in recirculating flow patterns, substantially altering reactive transport dynamics [3-4]. Thus, non-linear effects may have significant implications for pore-scale mineral dissolution. However, the effects of fluid inertia and 3D flow on pore-scale mineral dissolution, as well as their impact on upscaled processes, remain largely unknown.

In this study, we investigate the effects of fluid inertia and 3D flow on mineral dissolution using milli-fluidic experiments and pore-scale numerical simulations. We conduct laboratory dissolution experiments with a real-time imaging system and a rock analog material, and we perform pore-scale

reactive transport simulations using a micro-continuum approach to capture spatiotemporal evolution of a mineral phase due to dissolution. Both experimental and simulation results demonstrate the importance of fluid inertia in governing dissolution patterns. For example, along the mean flow direction, we find that low inertia induces fast dissolution on the inlet side, while the high inertia case exhibits the opposite effect (Figure (a)). In addition, distinct dissolution patterns, such as bifurcated in low inertia and concave in high inertia, appear on the mineral surface in 3D (Figure (b)). We conduct a detailed flow topology analysis and find that changes in the topological properties of 3D flows under varying inertia regimes predominantly control the formation of these distinct 3D surface patterns, which cannot be captured in 2D studies. Finally, we analyze the implications of these 3D dissolution dynamics on the upscaled relationship of porosity and reactive surface area; the analysis shows similar trends between the 2D cases and a conventional relationship, while the 3D cases significantly deviate from it. Our study highlights the significance of fluid inertia and 3D flows on pore-scale mineral dissolution and their implications on Darcy-scale processes.

Country:

United States

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MS25 / 169

Impact of Fluid Inertia on Mixing-Induced Mineral Precipitation: Pore-Scale Simulations and Microfluidic Experiments

Authors: Woonghee Lee¹; Fengchang Yang²; Vitalii Starchenko³; Xiaoru Liu¹; Peter Kang¹

¹ *University of Minnesota*

² *Chinese Academy of Sciences*

³ *Oak Ridge National Laboratory*

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Mineral precipitation induced by the pore-scale mixing of fluids with different reactants plays a vital role in various subsurface processes and applications, such as carbon mineralization, contaminant transport, and hydrogen storage. During in situ carbon mineralization, the mixing between injected carbonated water and ambient groundwater may lead to rapid mineralization. Most previous studies on mixing-induced mineral precipitation in porous media systems have focused on Stokes flow regimes, while recent studies have highlighted the importance of fluid inertia in these systems. Chen et al. (2024) show that fluid inertia enhances mixing in porous media by inducing recirculating flows [1], and Yang et al. (2024) demonstrate that fluid inertia controls mixing dynamics at channel intersections, leading to dramatic variations in precipitation patterns [2]. However,

the role of fluid inertia in mixing-induced mineral precipitation in porous media and its impact on upscaled processes remain largely unexplored.

In this study, we combine microfluidic experiments and pore-scale numerical simulations to investigate how fluid inertia influences mixing-induced mineral precipitation and the upscaled relationship. We conduct mineral precipitation experiments in microfluidics and perform pore-scale reactive transport modeling using a micro-continuum approach. The model captures the spatiotemporal variation in mineral precipitation governed by nucleation and growth processes. The nucleation process is described by Classical Nucleation Theory, and the growth process is governed by the rate law of Transition State Theory. Simulation results at 1,000 pore volume injection (PVI) show that precipitation occurs along the narrow mixing interface in the low inertia regime at $Re = 1$ (Figure (a)). In contrast, in the high inertia regime at $Re = 100$, the emergence of recirculating flows across the porous media induces vigorous mixing, resulting in precipitation over a wider area (Figure (b)). Simulation results are analyzed to identify the upscaled reactive surface area-porosity-permeability relationship under different inertia regimes. Our study highlights the significance of inertial flows in pore-scale mineral precipitation and their implications for carbon mineralization and clogging.

Country:

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[1] Chen, M. A., Lee, S. H. & Kang, P. K. Inertia-induced Mixing and Reaction Maximization in Laminar Porous Media Flows. *Proc. Natl. Acad. Sci.* 121, e2407145121 (2024). [2] Yang, W., Chen, M. A., Lee, S. H. & Kang, P. K. Fluid inertia controls mineral precipitation and clogging in pore to network-scale flows. *Proc. Natl. Acad. Sci.* 121, e2401318121 (2024).

MS13 / 170

Bound water transport by diffusion in wood revealed by Nuclear Magnetic Resonance

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Wood's unique combination of low density, high strength and stiffness, low thermal and electrical conductivity makes it versatile across diverse fields such as construction, furniture making, wood-carving, tooling, sculpture, boat building, along with production of cellulose fibers and paper. However, as a hygroscopic material, the water content and transport within wood strongly affect the structural performance of wood across diverse contexts. Therefore, understanding the physical mechanisms underlying water transfer processes in wood is crucial for optimizing its applications. This appears challenging considering that wood is a porous medium containing water in a range of pores of size from about 100 microns to less than a nanometer, i.e., the bound water, which plays

a fundamental role in water transport in wood [1-2]. Here we present a unique set of results concerning imbibition and drying of wood which allow to fully quantify the bound water transport properties.

Water imbibition within the microstructure of cubic samples was examined using nuclear magnetic resonance (NMR). Dynamic NMR relaxometry enables to differentiate the water in fibers, vessels, or as bound water in cell walls, enabling quantification of these water fractions over time. It was observed that water initially penetrates as bound water, followed by slower infiltration into fibers and subsequently into vessels, which exhibit the slowest rate of invasion. Given that bound water penetrates prior to free water, a global diffusion coefficient of bound water can be estimated based on measurements across different directions [3]. To further investigate the potential coupling between the invasion of various pore types, we isolated the diffusion of bound water by saturating the sample vessels with oil. Remarkably, our measurements show that the diffusion coefficient of bound water alone is independent of the water content, independent of the direction through the wood, almost independent of the wood species, and varies exponentially with the inverse of the temperature, suggesting that bound water diffusion behaves as an activated process.

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Water & Porous Media Focused Abstracts:

This abstract is related to Water

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MS06-B / 171

Stochastic modeling of reaction at the fluid-solid interface

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Understanding, quantifying, and predicting biogeochemical reaction rates is a fundamental scientific challenge with broad implications for the characterization and management of the critical zone and beyond. Unlike under the special conditions found in laboratory batch tests, mass transfer limitations are ubiquitous in natural systems, and the resulting incomplete mixing that can dramatically affect reaction rates. Reactive transport modeling is therefore a necessary tool for understanding these systems. In particular, stochastic approaches provide us with a framework to quantify the role of heterogeneity under incomplete information about medium structure and spatial reactant distributions.

This talk will cover theoretical and numerical stochastic approaches to quantify and upscale pore-scale reaction rates under advection and diffusion in heterogeneous porous media. The focus will lie on fluid-solid, or heterogeneous, reactions, which take place between dissolved species transported

by the fluid phase and solid-phase species found at the fluid-solid interface. From a theoretical standpoint, I will introduce the link between incomplete mixing, inter-reaction times, and first passage times, and how it can be quantified within a continuous time random walk framework. In terms of numerics, I will present particle tracking methods and their application to the direct simulation of reactive transport and the quantification of reaction rates from first passage times. Throughout the talk, I will discuss how these theoretical and numerical approaches help us shed light on the impact of medium and flow structure on reaction rates under both saturated and partially-saturated conditions.

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MS20 / 174

Effects of Fracture-Matrix Flow Interactions on Biofilm Formation in Rough Fractures

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Biofilms, aggregates of microbes, play a crucial role in subsurface processes and applications, including groundwater contamination and remediation, as well as biomineralization. In fractured media, fluid flow predominantly occurs through fractures due to their higher permeability compared to the surrounding rock matrix. The rock matrix, on the other hand, stores most of the fluid and provides significant storage capacity. The effects of fluid flow on biofilm formation have been studied, revealing that biofilm formation can significantly alter flow paths and even clog them, thereby affecting the permeability of the medium. Recent studies also show that fluid exchange between the matrix and fractures can significantly influence solute transport, implying the potential importance of fracture-matrix flow exchange on biofilm formation within fractures. For example, nutrient exchange between the surrounding matrix and fractures can potentially control the growth pattern of biofilm. However, the interplay between fracture flows, matrix effects, and biofilm formation in fractured media remains poorly understood.

This study aims to provide a comprehensive understanding of the mechanisms of biofilm formation in fracture-matrix systems by utilizing our recently developed pore-scale micro-continuum numerical model for biofilm formation [1]. We compare biofilm formation under fluid flow and nutrient transport across various fracture-matrix configurations, including a single fracture with an impermeable matrix and a fracture with a matrix of different permeability levels. Additionally, we investigate the effects of fracture roughness and flow rates on flux exchange between the fracture and matrix, as well as their impact on biofilm growth. The interplay between biofilm formation, channel flows, and matrix effects is quantified through the first passage time distribution, velocity distribution, and biofilm growth rate over time. The simulation results highlight the critical role of matrix effects on

biofilm formation in fractured media, providing scientific evidence for potential applications such as bioremediation in fractured rock aquifers.

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MS25 / 176

Assessment of Hydrodynamic and Geochemical Controls on Carbon Mineralization Process in Mafic and Ultramafic Rocks

Authors: Lawrence Opoku Boampong¹; Jeffrey D. Hyman¹; Alexander C. Murph¹; William J. Carey¹; Alexis r Navarre-Sitchle²; Hari S. Viswanathan¹

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One promising proposed strategy to reduce the CO₂ level in the atmosphere is inject it into the sub-surface and permanently trap it via geochemical reactions, where the CO₂ reacts with the formation to precipitate carbonate minerals (i.e., carbon mineralization). While the total amount of mineralized carbon depends on coupled processes: chemical, hydrological, mechanical, and thermal, the relative sensitivity of the mineralization extent with respect to the changes in these parameters is poorly understood. By utilizing advanced simulation techniques, this study aims to quantify the effects of various variables on the carbon mineralization extent in mafic and ultramafic rocks, thereby enhancing our understanding of geologic CO₂ sequestration in these systems. The results indicated that the initial porosity and temperature showed the strongest impact on the maximum amount of carbon mineralization in this system.

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MS05 / 177

Hydraulic boundary conditions control feedbacks between fluid flow, biofilm growth, and dissolved oxygen in groundwater**Author:** Hamidreza Ahadiyan¹**Co-authors:** Jason Mick¹; Arunima Bhattacharjee²; Eleanor Fadely³; Veronica Morales³; Jasquelin Pena³; Kevin Roche¹¹ *Boise State University*² *Pacific Northwest National Laboratory*³ *University of California, Davis***Corresponding Authors:** pena@ucdavis.edu, ecfadely@ucdavis.edu, vermoraes@ucdavis.edu, kevinroche@boisestate.edu, hamidrezaahadiya@u.boisestate.edu, arunimab@pnnl.gov

Biofilms are sediment-attached microbial communities that fuel numerous reactions in groundwater. Biofilm clogging of pores, or bioclogging, instigates dynamic feedbacks between fluid transport, oxygen demand, and microbial growth and decay that are poorly understood. Here, we present results from microfluidic experiments to demonstrate that these feedbacks are controlled by the hydraulic conditions driving flow. The microfluidic chambers (micromodels) were patterned after a homogenous sand and integrated with an optode sensor to measure dissolved oxygen (DO). *Bacillus subtilis*, a model biofilm-forming soil bacterium, was grown by flowing an oxygenated nutrient-rich solution through the micromodel. Two types of experiments were conducted, each with identical initial conditions but different boundary conditions: constant flow rate (Q) vs. constant pressure gradient (ΔP). Bulk permeability was quantified over time by relating measured flow and pressure to Darcy's Law. Microscopy was used to monitor spatial maps of biomass and DO.

For both conditions, biofilm patches formed uniformly at early times. Coalescence of patches caused permeability to decrease 30-fold and average DO to decline to anoxic conditions (i.e., DO <2 mg/L) in the first 24 h. Distinct pseudo-steady state behavior emerged over the remainder of the 48 h experiments that differentiated the two boundary conditions. Experiments at constant Q promoted frequent permeability fluctuations and flow channelization into preferential flow paths (PFPs) that maintained a fully connected pore network. DO concentrations correlated strongly with PFP location, with concentration declining along PFPs and spatial maps of DO responding to changes in PFP location. In contrast, biofilm fully clogged pores near the micromodel inlet in constant ΔP experiments, which restricted DO availability and caused biofilm to slough in DO-depleted locations. Sloughing was followed by a regrowth period characterized by slow changes to permeability, biomass, and bulk DO. Our results demonstrate that hydraulics fundamentally control the dynamics of bioclogging and therefore determine the spatio-temporal heterogeneity of redox conditions that determine the transformation of redox-sensitive elements in groundwater.

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MS25 / 179

pH-Driven Mixing-Induced Carbonate Mineralization: Insights from Microfluidic Pore-Scale Experiments

Authors: David Kyungtae Kim¹; Peter Kang²

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During in situ carbon mineralization, the mixing of injected carbonated water with ambient groundwater can trigger rapid mineral formation. Notably, pH strongly influences carbonate speciation, which is pivotal in driving carbon mineralization. Previous studies have shown that when two fluids mix and create a supersaturated environment with respect to certain minerals, precipitates form at the mixing boundary, resulting in a thin barrier that impedes further mixing over time. However, mineral precipitation can also occur through pH-driven speciation changes during neutralization reactions, particularly when the speciation of mineral constituents depends on pH (e.g., CO_3^{2-} to HCO_3^-). Despite its importance, pH-driven precipitation in the context of pore-scale carbon mineralization has not been investigated. This study investigates the pH-driven carbon mineralization during the mixing of alkaline groundwater and carbonate-rich water.

The microfluidic experimental setup mimics downstream environments in geological carbon sequestration, where the injected carbonate-rich fluid approaches equilibrium with respect to calcite, and OH^- diffusion occurs from the surrounding matrix. To achieve this, we injected a CaCl_2 solution adjusted to pH 11 and a CaHCO_3 solution, slightly undersaturated with respect to calcite at pH 6.5, into separate inlets of a porous microfluidic device using a syringe pump, while maintaining the same Ca^{2+} concentration on both side. The flow rate was varied to assess its impact on the precipitation, with changes in flow rate altering the Peclet number of OH^- from 0.19 to 13 and HCO_3^- from 0.84 to 58. The results revealed that the precipitation band was markedly shifted toward the carbonate-rich side (Figure). As the Peclet number (Pe) increased, the precipitation band narrowed, although it consistently formed on the carbonate-rich side. A parallel experiment mapping pH using a pH-sensitive fluorescent dye revealed pH changes at the interface where the two fluids mixed, aligning with the location of the precipitation band. This shift in the precipitation band is driven by the faster diffusion of OH^- , which induces deprotonation from HCO_3^- to CO_3^{2-} . The Grotthuss mechanism explains this rapid diffusion of OH^- ions, distinguishing them from typical solutes dissolved in water. This accelerated diffusion plays a critical role in facilitating the observed shift in precipitation band by enhancing local pH changes and carbonate availability. The corresponding results were modeled using COMSOL, demonstrating good agreement with the experimental observations. This study reveals the importance of considering mixing-driven carbon mineralization especially in the context of pH sensitive reactions. The work has implications to flow channel clogging during mineralization and offers a potential explanation for the formation of veins in geological formations.

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MS10 / 180

Tracking rock dissolution with synchrotron-based high-speed, high-resolution 4D X-ray tomography

Authors: Michał Dzikowski¹; Piotr Szymczak¹

Co-authors: Marta Majkut²; Tymoteusz Kosiński³; Dawid Woś¹

¹ *Faculty of Physics, University of Warsaw*

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During the flow of a matrix-dissolving fluid through porous media, positive feedback between flow and reaction generates diverse, evolving structures [1]. These range from intricate, cave-like wormholes to simple surface dissolution patterns. The dynamics of this hydrochemical instability depend on both flow rate and the geometric properties of the pore space. While the effects of flow and reaction rates on wormhole formation are well established [2], the mechanisms governing their propagation dynamics remain poorly understood.

This study investigates the fast-progressing dominant wormhole regime, which has applications in various industrial and natural contexts, including carbon capture and storage. Understanding the dynamics of fluid interaction with the porous matrix requires high-resolution temporal and spatial data. We have recently conducted in-situ X-ray micro-CT imaging of developing wormholes in dissolving limestone cores flooded with hydrochloric acid, achieving high temporal frequencies (50–100 frames per experiment) [3]. To further improve temporal and spatial resolution, we utilized the ID-19 beamline at the European Synchrotron Radiation Facility. A limestone core was confined in a Hassler cell and flooded with hydrochloric acid, while high-frequency 4D tomographic data tracked the evolving 3D shape of the growing wormhole. The time evolution of the wormhole profile has been compared with an analytical model of the growth of the tube-like dissolution structure [4]. As we show, such data, when properly interpreted, allow for a measurement of the mineral dissolution rate constant and the assessment of the impact of diffusive transport on the dissolution process.

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Variations in 3D Biofilm Growth Patterns Under Anaerobic and Aerobic Growth Conditions

Authors: Dorte Wildenschild¹; Julia Lauterbach¹; Tala Navab-Daneshmand¹

Co-authors: Alice Bokman¹; Laura Osborne¹; Mads Kent¹; Margaret Robinett¹

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Biofilm formation in porous media is crucial for understanding microbial processes in subsurface environments, bioremediation, and engineered systems. Previous research has shown that growth may be oxygen-limited under slow flow rates when oxygen is the sole electron acceptor (i.e. under aerobic conditions). Our current research involves growing biofilms in micro-gravity on the International Space Station (ISS), where, due to volume constraints on the cargo shuttles, only a limited amount (volume) of nutrients can be transported to space. This study, therefore, explores the development of monoculture, *Shewanella oneidensis*, biofilm in porous media under varying growth conditions, using either oxygen or sodium nitrate as the terminal electron acceptor. Biofilms were cultivated in glass flow reactors (7 mm i.d.) packed with glass beads ranging in size from 650-1200 microns. Syringe pumps delivered prescribed nutrient volumes at controlled flow rates and elevated temperatures (38 °C) to produce ample growth. The goal was to compare growth and 3D biofilm architecture differences using the two electron acceptors.

The reactors were imaged using X-ray microCT to compare the two growth conditions, and the resulting data was processed with advanced image analysis software. Contrast agents were employed to differentiate the biofilm from the aqueous phase at the time of imaging. Deep learning algorithms were applied to segment the data into porous medium, biofilm, and aqueous phases. Several key metrics were analyzed to quantify the differences between the two growth scenarios, including biofilm volume, area, 3D distribution within the porous medium, and topological variables representing the connectivity of the biofilm.

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MS09 / 183

A variational phase-field model for porous ice and salty water interactions

Author: Junning Liu¹

Co-author: Xiaojing Fu¹

¹ *California Institute of Technology*

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Ocean-ice interactions, particularly the dynamics of melting and refreezing at the ice-ocean interface, are critical in determining ice shelf stability and predicting large-scale ice sheet behavior. These processes exhibit significant spatial and temporal heterogeneity due to the complex couplings among the transport of salinity and temperature fields, and density-stratified fluid flow. In this study, we use the phase-field method to model ice as a porous medium to more accurately capture its microstructural properties and the associated transport phenomena at the ice-ocean interface. The phase-field framework enables a robust, thermodynamically consistent representation of phase transitions between solid and fluid phases without requiring explicit interface tracking. While this technique has been used in recent years to model ice melting under turbulent flow, existing models often adopt a nonvariational formulation and focus on evolution of macroscopic ice-water interfaces (e.g., cm to m scale).

In this work, we develop a variational phase-field model based on a temperature-and-salinity-dependent Gibbs free energy functional of water-salt mixtures to describe the coupled interactions between porous ice and salty water at the pore scale (e.g., μm to cm). The functional is formulated to recover the phase diagram of seawater in the -10°C to 0°C range, capturing the equilibrium phase diagram as controlled by the bulk salinity and temperature of the system. By incorporating diffusion, advection, interfacial effects, and phase transition dynamics via the Allen-Cahn and Cahn-Hilliard evolution equations, the model predicts the co-evolution of the phase field, salinity, temperature, under laminar flow. We present high-resolution numerical simulations that illustrate the melting and refreezing dynamics under diverse environmental conditions, including varying flow configurations, salinity gradients, and temperature distributions. The model effectively resolves these dynamics within complex geometries in the mushy layer of the ice sheet and across different flow regimes. These results illustrate the intricate interplay of salinity, temperature and phase change in ocean-ice interactions, contributing to a more precise understanding of pore-scale mechanisms of mushy ice evolution and their impact on larger-scale ice sheet evolution under dynamic oceanic forcing.

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184

Study on the co- and counter-current spontaneous imbibition characteristics of ideal connected capillaries with unequal diameters

Author: Kangli Chen¹

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Spontaneous imbibition is widespread in both industry and nature. The pore size distribution in porous media has an important impact on imbibition. In this study, we developed a model consisting of five interconnected ideal capillaries to analyze spontaneous imbibition processes in porous media. In this model, both co- and counter-current are considered. By solving the mathematical models,

the advancement speed and position of the oil-water interface in each capillary were obtained. The calculation results indicated that the difference in the advancing distance of the oil-water interface fronts among different capillaries increases as the imbibition proceeds. As the oil-water viscosity ratio increases, oil production by counter-current imbibition increases, and the difference in the advancement distances of the imbibition front also increases, which is consistent with experimental conclusions. The distance difference in the advancement of imbibition fronts increases with greater variation in capillary diameters. However, when capillary diameter difference exceeds a certain threshold, the distance difference in imbibition front advancement begins to decrease as the capillary diameter difference further increases. These results will enhance our knowledge about the mechanisms of spontaneous imbibition.

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MS20 / 186

Investigating Drying Dynamics and Shrinkage in Biological Materials Using NMR Techniques: Potatoes as a Case Study

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Co-authors: Benjamin Maillet ¹; Philippe Coussot ²

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The drying of biological materials, such as vegetables and fruits, is a critical process in food preservation, enhancing shelf life, maintaining nutritional value, and reducing transportation costs. Potatoes, as a staple crop and a primary source of carbohydrates globally, are particularly significant in this context. However, drying processes for biological materials are often complex, involving coupled heat and mass transfer, non-linear shrinkage, and evolving pore structures. A deeper understanding of these phenomena is essential for optimizing drying techniques, minimizing energy consumption, and improving product quality.

In this study, we employ Nuclear Magnetic Resonance (NMR) techniques with home-made sequence [1] to investigate the drying dynamics and shrinkage behavior of potatoes. A NMR CPMG sequence is adopted to distinguish and track water states, which enables us to precisely distinguish three types water according to their different transversal relaxation times (T₂): intracellular free water, cell wall water, and bound water adsorbed in starch granules. As the drying rate on boundary may impact the drying mechanism [2, 3], one-dimensional drying experiments on cylindrical potato samples have been conducted. Under slow drying conditions, the drying rate remains constant while most of the water is extracted, then it starts decreasing. We show that during the constant rate period the free water is first extracted, then the cell wall water; the decreasing rate period corresponds exactly to the extraction of bound water. Under fast drying conditions, the drying rate continuously decreases, and T₂ signals corresponding to intracellular and cell wall free water diminished simultaneously,

with bound water drying occurring only after the disappearance of all free water and bound water. Interestingly, the drying rate decreased continuously from the beginning.

These results yield the complex interplay between water transport mechanisms and structural changes. Our findings suggest that intracellular free water may first transition to cell wall free water for effective transport and diffusion. Additionally, isotropic drying shrinkage was observed during initial drying, maintaining sample saturation. Anisotropic shrinkage appears once longitudinal shrinkage reached a threshold. As drying progressed, voids pore emerged, facilitating water vapor diffusion, indicating a shift from liquid (bound) water transport to combined liquid (or bound water)-vapor transport in later stages. A similar phenomenon of bound water-vapor transport was observed in our previous work [4]. Based on our experimental observations, we propose a comprehensive physical model to describe the coupled processes of drying-induced shrinkage, water transport, and vapor diffusion. This model provides a robust framework for advancing drying technologies in food science and material engineering.

The implications of this study extend beyond potatoes to other fruits and vegetables, offering insights into the optimization of drying processes across a range of agricultural products. Improved understanding of these dynamics can lead to energy-efficient drying techniques, reduced food waste, and better preservation of quality and nutritional content. These outcomes are particularly critical in the context of global food security and sustainability.

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Logging curve reconstruction based on the Improved Transformer Neural Network Model

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Logging curves are crucial data in geophysical exploration, reflecting the stratigraphic structure and reservoir characteristics. However, due to various factors and equipment failures during drilling, logging curve data often present issues with missing values and noise. Currently, traditional machine learning-based methods for logging curve reconstruction fail to account for correlations within the

depth space of well logging curves. To address these issues, we propose a deep learning based surrogate model, improved from the transformer neural network (T-NN). Case studies are performed to investigate the performance and generalization of this surrogate model named improved transformer neural network (IT-NN). The results indicate that the proposed surrogate model based on IT-NN can be used for logging curve reconstruction accurately and robustness. This provides a novel approach for data analysis in geophysical exploration.

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MS10 / 188

Tomographic analysis of surface reactivity and transport

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Co-authors: Jann Schöngart¹; Johannes Kulenkampff¹

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Tomographic flow field analysis using positron emission tomography (PET) has become an important method for identifying pore-scale heterogeneities. Diffusive flux [1] and advective transport [2] can be quantified using conservative tracers, and even local flow field changes due to reactions such as dissolution or precipitation can be quantitatively characterized. Reactive tracers, in comparison, can provide quantitative information on the evolution of surface reactivity. In particular, sorption and desorption reactions at material surfaces are examined with temporal and spatial resolution [3]. Here we focus on the varying surface reactivities of crystalline materials as a function of their nanoscale properties, i.e. surface nanotopography and reactive site density. We discuss the use of various PET tracers and highlight their applicability for reactive transport studies. Conclusions from these investigations provide quantitative insights into important applications, including the fate of contaminants in the subsurface, remediation reactions, and nuclear waste repositories.

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Evaluation method of multilithologic stratified shale reservoirs based on equivalent macroscopic mechanical properties

Authors: Gongchen Yang¹; Shuang Liang¹

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Stratified shale reservoirs are characterized by complex lithology, great differences in mechanical properties and ground stresses, and the key to successful fracturing of shale reservoirs is to master the law of reservoir fracture penetration with interlayers. Considering rocks as composite materials composed of various minerals, representative volume elements (RVE) containing different mineral properties are introduced. The equivalent macroscopic mechanical parameters of rocks are solved through the finite element platform with periodic boundary conditions and verified. A multi-lithology layered shale reservoir model is established. Based on the predicted mechanical properties of different lithology rocks by the equivalent macroscopic mechanical property characterization method, numerical simulation studies on the propagation of hydraulic fracturing fractures are carried out, comprehensively considering several influencing factors such as vertical stress of the reservoir and interlayer, fracturing fluid flow rate, fracturing fluid viscosity, and brittleness mineral index. The effective connected area of fracture height is introduced, and a multi-lithology reservoir cross-layer effect evaluation method considering reservoir and interlayer properties as well as construction parameters is established by using the fuzzy analytic hierarchy process. The results show that the vertical stress, interlayer stress and brittleness index of interlayer are negatively correlated. Fracturing fluid displacement and fracturing fluid viscosity are positively correlated with fracture growth. Based on the changes of fracture propagation by various factors, the identification criteria of effective reservoir propagation can be established to predict and control fracture propagation more effectively, so as to improve the mining efficiency and economic benefits of multi-lithologic stratified shale reservoirs.

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Quantification of Pore Diameter in Solder Joints of Printed Circuit Boards Based on Super-Resolution Microcomputed Tomography

Author: Sascha Senck¹

Co-authors: Julia Maurer¹; Lukas Behammer¹; Lukas Nepelius¹; Miroslav Yosifov¹; Patrick Weinberger¹

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Non-destructive characterization of printed circuit boards (PCBs) is crucial for ensuring the reliability of electronic components. Defects like cracks and pores in solder joints significantly influence the performance of PCBs. Microcomputed tomography (μ CT) has proven effective in detecting such pores and quantifying relevant characteristics like diameter, volume, and shape. The current study expands on these findings by introducing super-resolution (SR) μ CT, utilizing a novel approach that integrates μ CT imaging with convolutional neural networks (CNN) for resolution enhancement. Using SR μ CT and a pre-trained CNN, it is possible to generate high-resolution (HiRes) image data from low-resolution (LowRes) input data that was not part of the training cohort. This methodology bridges the gap between high-throughput imaging and detailed pore characterization, since LowRes μ CT scans can be carried out several times faster.

In this contribution, 18 PCB samples featuring a total of 432 solder joints were scanned at a voxel size of 8 μ m to create a high-resolution (HiRes) reference dataset using a Nanotom 180 system. Voltage was set to 140 kV using an integration time of 650ms and 1800 projections resulting in a total scan time of 19min per sample. We focus on developing a methodology to generate corresponding LowRes datasets directly from HiRes scans using different downsampling approaches, e.g. topology-guided downsampling and edge-preserving downsampling, followed by image filtering approaches like Gaussian blur. Our goal is to generate realistic LowRes image data that resembles actual LowRes μ CT data. In order to check the feasibility of artificially generated LowRes data for training, downsampled data was compared with actual LowRes μ CT scans (voxel size: 40 μ m) of the same sample using structural similarity index (SSIM) and feature similarity index (FSIM). Preliminary results show a high SSIM of 0.91 between the compared data sets.

Artificially downsampled and filtered data was subsequently used in our SR approach that employs a U-Net 3D architecture augmented with LossNet [2]. The model was trained using paired HiRes and LowRes datasets to predict high-fidelity 3D pore maps from LowRes inputs. Evaluation metrics included SSIM and peak signal-to-noise ratio (PSNR).

At 8 μ m voxel size, diameters of detected pores in HiRes data vary between 27 μ m and 235 μ m. Preliminary results show that SR images provide a more precise estimation of maximal pore diameter compared to LowRes data. However, small pores with a diameter below ca. 60 μ m are not detected. Nevertheless, since the smallest pores detected in LowRes data have a diameter larger than 120 μ m, this is a significant improvement in defect detectability. One advantage is the increase in scan speed, since LowRes scans were carried out in 5 min compared to 19 min total scan time of the respective HiRes scans. Our work focuses on the determination of the optimal downsampling approach and the effect of the choice of training samples on the prediction probability. In future, we will diversify the training sample for a generalized model for various porous media.

Acknowledgements

This work is funded by the IBW/EFRE & JTF project "HyperMAT" (Österreich 2012-2027) and the FFG project "sustainDT" (909801).

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MS11 / 191

Investigation of dissolvable gases transport in vadose zone by using micromodel experiments**Authors:** Yung-Wei Lee¹; Kai-Xiang Zhan¹; Qun-Zhan Huang¹; Shao-Yiu Hsu¹¹ National Taiwan University Department of Bioenvironmental Systems Engineering**Corresponding Authors:** kevin90836@gmail.com, s95568teresa@gmail.com, syhsu@ntu.edu.tw, qzhuang1024@gmail.com

Dissolved gases in soil pores play a crucial role in soil pollutant transport, subsurface carbon sequestration, and soil greenhouse gas emissions. The transport of dissolved gases interacts with trapped soil air. Trapped air in soil impedes the transport of dissolved gases in porous media. Meanwhile, the exchange of dissolved gases between liquid and gas phases alters bubble volume and surface area, thereby changing the exchange characteristics of dissolved gases and the migration of bubbles.

Although previous studies have explored the interactions between dissolved gases and trapped air bubbles, soil air not only exists as trapped bubbles but also includes free air connected to the atmosphere (e.g., in the vadose zone). Compared to the former, the latter exists under low water content. The transport behavior of dissolved gases differs between these two types of soil air. Furthermore, the behavior of dissolved gas transport under significant variations in water content remains one of the unresolved research challenges.

Through experiments using micromodels with simple and complex pore structures, we quantified the effects of free air on trapped bubbles. Simple pore experiments examined the influence of increasing the number of trapped bubbles on gas diffusion and how the size of trapped bubbles changes with injection rates. Experiments involving lotus root-like flow channels investigated bubble formation and size. Complex pore micromodels were used to explore the differences in bubble trapping and movement with and without dissolved gases.

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References:

MS10 / 192

Study of Corrosion Behavior in Wellbore Cement Containing a Leakage Pathway under different Acidic Conditions**Author:** Manguang Gan^{None}**Co-authors:** Liwei Zhang¹; Yan Wang¹; Yue Yin¹; Hanwen Wang¹

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During the process of geological CO₂ storage, the injection of CO₂ can lead to the creation of a reservoir environment enriched with carbonic acid. If the reservoir brine contains high concentrations of chloride (Cl⁻) and sulfate (SO₄²⁻) ions, low-pH environments rich in these ions may also develop. Assessing the risk of CO₂ leakage through internal cracks in wellbore cement necessitates a detailed analysis of morphological changes in cement containing leakage channels before and after exposure to various acidic conditions. This study examines the morphological and structural alterations in wellbore cement with leakage channels before and after the following of CO₂-saturated brine, and compares these changes to those observed after exposure to hydrochloric acid (HCl) and sulfuric acid (H₂SO₄) solutions. The findings reveal that cement surrounding the leakage channel undergoes dissolution, resulting in an increase in channel volume when exposed to CO₂-saturated brine. This reaction is more pronounced at the inlet end compared to the outlet end, accompanied by the formation of cracks in the vicinity of the channel. As HCl solution flows through the channel, a hydrate precipitate containing calcium and aluminum forms from the inlet to the middle, attributed to the mixing of aqueous phase cations (Ca²⁺ and Al³⁺ released from hydrated cement phases) with high-pH pore fluid ahead of the acid front. Upon exposure to H₂SO₄ solution, a thin precipitation layer forms at both the inlet and outlet ends of the channel, composed of gypsum (CaSO₄·2H₂O) as indicated by X-ray diffraction (XRD) analysis, resulting from the reaction between SO₄²⁻ in the acid solution and Ca²⁺ in the cement hydration product. Following exposure to HCl and H₂SO₄ solutions, the channel volume decreased, suggesting that secondary precipitation from the cement-acid reaction surpassed cement dissolution, limiting the expansion of the wellbore cement's internal channel in hydrochloric and sulfuric acidic environments. The experimental results further indicate that, within acidic environments of equivalent pH, CO₂-saturated brine exhibits the highest corrosivity towards wellbore cement, followed by hydrochloric acid, with sulfuric acid demonstrating the least corrosive.

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MS10 / 193

Experimental investigation on H₂S-induced oilwell cement degradation under high-temperature conditions

Author: Yue Yin¹

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Oilwell cement is a weak point in wellbores used for extracting geothermal resources. It can be corroded by acidic gas such as H₂S under high-temperature. Previous studies have primarily focused on the immersion corrosion or one-phase corrosion of oilwell cement in H₂S solutions, while corrosion

along existing cracks requires attention. Given this, this study conducted experiments on the corrosion of H₂S solution along channels within oilwell cement using a high-temperature-high-pressure flow reactor. The structural evolution of the cement under H₂S corrosion was evaluated using CT scanning, while SEM and XRD tests were used to provide a micro-level mechanistic explanation. The results indicate that H₂S corrosion leads to a decrease in the strength of oilwell cement and an increase in permeability. During H₂S induced corrosion along the channel, the porosity of the cement increases, with the formation of more macro-pores. The wall of the channel undergoes chemical dissolution and roughening, leading to an enlarged channel. The dissolution of primary minerals of the cement and the formation of secondary minerals such as pyrite are believed to destabilize the microstructure.

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194

Research on the laws of carbon dioxide sequestration, storage, and transportation in saline aquifers, as well as factors affecting the storage capacity.

Authors: Shangkun Chen¹; Liyan Sun¹

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Calculate the storage capacity and study the mechanism of carbon dioxide sequestration by constructing sequestration, dissolution sequestration, residual gas sequestration, mineralization sequestration, etc. Design the effects of different well types, injection well depths, injection rates, injection volumes, injection pressure differentials, and other parameters through physical models and numerical simulation methods.

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MS03 / 198

Transmissibility Upscaling in Karst Carbonate Rocks Using Surrogate Models

Author: Patricia Pereira¹

Co-authors: Marcio Murad²; Tayná Lobo³; Emanuel Lourenço³

¹ *Laoratório Nacional de Computação Científica*

² *Laboratorio Nacional de Computacao Cientifica*

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Corresponding Authors: tlobo@lncc.br, egomes@lncc.br, murad@lncc.br, patricia@lncc.br

We developed a new methodology to compute hydraulic transmissibility between karst-conduits and rock matrix in carbonate reservoirs. Such a parameter quantifies the mass exchange between these two geological objects and can be explored in EDKM-type models (Embedded Discrete Karst Model) via non-neighboring connections. The upscaling procedure adopted hinges on the karst index concept, whose underlying physics relies on the generalization of the traditional Peaceman's theory of well index to more complex scenarios of coupled flow in karst conduit systems displaying general non-circular cross sections. Within the proposed procedure, we adopt the flow-based upscaling method to compute mass transfer between conduits and matrix for several configurations of conduits lying within cells of a coarse grid. The corresponding transmissibility value associated with each scenario is stored in a database. Subsequently, a machine learning model is trained on the numerical results in the dataset, using information related to the geometry of the karst-conduits as input attributes, and the transmissibilities computed with numerical simulations as target values. Numerical experiments are carried-out exhibiting the magnitude of the transmissibility for certain conduit arrangements, along with the magnitude determined by the machine learning algorithm. The results illustrate the potential of the methodology proposed herein. The novel approach can be applied to both aquifers and carbonate reservoirs, providing more accurate predictions and enhancing the management of such resources.

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MS07 / 199

Coupled Hyperbolic Approach to Solve Buoyant Two-Phase Flow and Transport in Heterogeneous Porous Media

Author: Armin Riess¹

Co-author: Patrick Jenny

¹ *ETH Zürich*

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Recently, a new approach for simulating buoyant two-phase flow and transport in porous media, which is based on a coupled hyperbolic system, was proposed. This new scheme incorporates Darcy's law by adding a source term to the isothermal Euler equations plus an extra equation for phase transport. The system allows for explicit computations and is solved in its hyperbolic form with a characteristics based Riemann solver. Thus, since all required operations are local, for many problems this method has significant advantages over previous ones in terms of computational cost and parallelizability.

Here, this approach is generalized for heterogeneous porous media, which has implications for the numerical solution algorithm. In particular, it is crucial that the source terms are considered by the Riemann solver, otherwise the results get contaminated by numerical errors. To achieve this, a new Rankine-Hugoniot-Riemann (RHR) solver is devised. It accounts for the source terms by introducing consistent Rankine-Hugoniot jumps in each finite volume cell (separately in all coordinate directions) while still honoring conservation.

Numerical results confirm that the new RHR solver is effective and that the explicit hyperbolic solution approach to coupled buoyant flow and transport in heterogeneous porous media is computationally efficient and leads to accurate results.

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Poster / 200

Role of Surface Roughness and Fracture Aperture in Enhancing CO₂ Mineralization in Synthetic Olivine Fractures

Author: Yun Yang¹

Co-authors: Chelsea Neil¹; Hari Viswanathan¹

¹ *Los Alamos National Laboratory*

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In-situ mineralization provides a promising pathway for permanent carbon storage, but achieving efficient subsurface mineralization requires sufficient permeability in the host rock formation, a significant challenge for scaling up these processes. This work investigates the effects of fracture characteristics (i.e., surface roughness and fracture aperture) on CO₂ mineralization reaction by reacting saw-cut dead-end fractures in forsteritic olivine. Synthetic fractures with controlled apertures (0.5–1.6 mm) and varying surface roughness were subjected to high-pressure (13.7 MPa) and high-temperature (185°C) CO₂ batch experiments for two weeks. Post-reaction characterization techniques, including Raman spectroscopy, X-ray diffraction (XRD), and optical microscopy, were used to assess the extent of mineralization, identify secondary minerals, and determine their relative abundance.

In small fractures (0.5–0.6 mm), results from optical microscopy and Raman spectroscopy showed

that the co-precipitation of magnesite (MgCO_3) and maghemite (Fe_2O_3) occurred primarily on rough surfaces, while smooth surfaces exhibited lower carbonation rates and minimal iron oxide precipitation. We also observed the diminishing effect of surface roughness on mineralization in large fractures (1–1.6 mm), as they exhibited more uniform magnesite and maghemite precipitation across both rough and smooth surfaces. This uniformity can be attributed to the formation of a Fe-Si-rich coating on the olivine surface. This coating masks the surface characteristics of the olivine, reducing the influence of surface roughness on carbonation rates. In smaller fractures, fewer ferrous oxides precipitate, leaving more olivine exposed to aqueous fluids. This exposure allows surface roughness to play a more significant role in influencing carbonation in smaller fractures.

This study provides fundamental insights into the effect of fracture characteristics on CO_2 mineralization. Understanding this relationship is essential for optimizing subsurface mineralization processes and scaling up operations to achieve meaningful contributions to carbon storage efforts.

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MS01 / 202

Wettability alteration of microfluidic devices by *in situ* plasma

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In this work, we propose a new method based on *in situ* plasma treatment to alter the wettability of microfluidics devices. The targeted contact angle remains stable for several days, offering new possibilities for investigating multiphase flow in porous media. Moreover, we demonstrate the influence of wettability alteration on two-phase flow and transport properties.

Microfluidics contributes to a better understanding of the multi-scale and multi-physics processes in geological environments. For example, the success of a secure and permanent storage of CO_2 in subsurface formations depends largely on our knowledge of two-phase fluid displacements and interphase mass transfer leading to residual saturation and dissolution of CO_2 . In these multi-fluid flow problems, a complex interplay of physico-chemical factors controls the fluid displacements, trapping, dissolution, and remobilization. The wettability is one crucial parameter that affects residual trapping and interphase mass transfer. Although the importance of wettability on multiphase flows and mass transfer is recognized, there is a lack of reliable and high-resolution data on its influence.

We developed a new method based on plasma treatment to control the wettability of microfluidic devices. Plasma is a promising tool, yet its propagation in microchannels and the stability of the treatment have remained challenging. This work aimed to produce and propagate an atmospheric pressure helium plasma directly into a closed microfluidic device made of glass for *in situ* treatment.

Results obtained through contact angle measurements within the microchannels demonstrated a uniform wettability treatment with increased hydrophilic properties after only 1 minute of plasma treatment. We studied the stability of the plasma treatment by storing the devices either in water or air and measuring the evolution of the contact angle with time. With storage in air, we achieved at least 1 day of stable contact angle at around 23°, while water storage prolonged this stability for up to 3 days. Storage in air resulted in a full recovery of the initial wettability state after 13 days. When devices are stored in water a partial loss of wettability is observed, leading to a new wetting condition at a contact angle of around 30° that is stable up to a remarkable 70 days. Contact angle results are further supported with X-ray photoelectron spectroscopy surface analysis which revealed that the two effective mechanisms for wettability alteration are cleaning and surface functionalization. This in-house setup enables the processing of already bonded microfluidic devices providing treatment of all the inner microchannel walls. In addition, we are able to direct plasma propagation with electrode positioning, thus providing a way for selective wettability treatment of complex geometries.

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MS03 / 203

Statistical integro-differential fracture model (Sid-FM): An efficient approach to simulate expected flow in fractured sub-surface formations

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Information about sub-surface formations is typically scarce and plagued by uncertainties. Especially when dealing with fractured formations, this strongly impacts the predictive power of numerical simulations. Isolated fractures for example may represent long-ranging highly conductive flow conduits having a strong impact on flow and transport. Furthermore, as fractures can reach extensions similar to the size of the domain of interest, homogenization may not lead to satisfactory results. Alternatively, fracture-resolving Monte Carlo simulations are typically used. However, due to their high computational costs, usually only few fractures can be incorporated in comparison to realistic formations. Sid-FM, on the other hand, circumvents a fracture-resolving description, but determines the ensemble-averaged flow field directly by incorporating the non-local effect of extended fractures through kernel functions. In this work it is shown that different kernel functions can accurately capture the effects of different fracture distributions, shapes, and clusters of connected fractures. The results of Sid-FM are compared against fracture-resolving Monte Carlo simulations in a series of numerical experiments. It is demonstrated that Sid-FM can quickly and inexpensively produce accurate flow estimates.

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MS13 / 204

BlueMat: Water-Driven Nanoporous Materials

Author: Patrick Huber¹

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The exquisite diversity and functionality of biological materials is truly remarkable, especially since they are composed of a small set of abundant chemical elements. While engineering materials primarily require specific, often unsustainable, chemical compositions to realize their functions, nature achieves unparalleled functionality through optimized architectures that span multiple length scales. Water, with its ubiquity and unique structural dynamics, plays a pivotal role as a nanoscale “working fluid” in shaping the properties and functionality of nature’s materials. Here, I will introduce a novel class of sustainable, interactive materials that derive their functionality from the interplay between hierarchical structures of hard matter, including nanoporous solids and water. I will show how these “Blue Materials” can mimic natural processes such as water-driven mechanical actuation[], capillarity-driven water transport, and humidity-responsive coloration and light scattering. I will also highlight their potential for innovative applications, including electrical energy storage and generation, thus extending the functionalities observed in nature.

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References:

MS03 / 205

Analysis and Comparison of Natural and Induced Single Fractures for Caprock Leakage Assessment

Author: Sahyuo Achuo Dze¹

Co-authors: Tomos Phillips ¹; Reza Najafi-Silab ¹; Sarah Perez ¹; Tom Bultreys ²; Vladimir Novak ³; Christian Schlepütz ³; Veerle Cnudde ²; Florian Doster ; Kamaljit Singh ¹; Kevin Bisdom ⁴; Andreas Busch ¹

¹ *Heriot-Watt University*

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Accurately modelling fracture networks in low-permeability formations like caprocks requires an understanding of the complexity of a single fracture geometry and its impact on flow. Fractures are often oversimplified as planar, ignoring the variability that influences flow behaviour. Most fracture geometry research focuses on granites and sandstones, while caprock fractures remain underexplored due to sampling challenges.

This study explores geometric and hydraulic differences between natural (NFs) and induced fractures (IFs) in the same caprock formation, providing insights for fracture network modelling to predict caprock flow behaviour. Three NFs and two IFs were analysed from core plugs extracted from the Carmel Formation, a low permeability caprock in Utah. NFs are natural shear fractures, while IFs were induced during drilling or coring. High-resolution synchrotron computed tomography images (voxel size: 2.75 μm) were used to segment fracture void geometries, enabling the extraction of surface profiles and aperture measurements.

Aperture heterogeneity was quantified using the coefficient of variation (CV), and surface roughness assessed using the Root Mean Square gradient (Z2), Joint Roughness Coefficient (JRC), and Hurst Coefficient (H). Variograms analysed spatial correlation. Permeability was measured under 25 bar effective stress using Darcy's law, with experimental results compared to parallel plate model predictions to evaluate geometric variability.

Results show positively skewed aperture distributions for all fractures. NFs exhibit greater heterogeneity ($\text{CV} > 0.5$) and more spatially random apertures compared to IFs ($\text{CV} < 0.5$), which display more uniform distributions. Surface roughness metrics (H, Z2, JRC) and Power Spectral Density (PSD) analyses do not consistently differentiate fracture types. However, variograms reveal longer correlation lengths for NFs, indicating greater spatial variability when combined with CV.

While cubic law models predict similar permeabilities for both fracture types, experimental results deviate significantly—reducing by 1–2 and 3–4 orders of magnitude for IFs and NFs respectively—highlighting the importance of spatial variability, particularly in sheared NFs.

These findings emphasize the need to (i) consider fracture types in network models and (ii) incorporate spatial variability into flow models to improve predictions of caprock integrity and leakage potential. Future work will numerically evaluate two-phase flow to predict displacement dynamics, providing critical insights into fracture network and overall caprock flow performance.

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Investigation of Transport and Retention of a Novel Sub-microgel in Porous Media

Author: Junchen Liu¹

Co-authors: Baojun Bai¹; Thomas Schuman¹; Mingzhen Wei¹

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Sub-microgels, crosslinked polymer particles, have attracted increasing interest in Enhanced Oil Recovery (EOR), Enhanced Geothermal System (EGS), carbon storage, and groundwater management field. However, it is still unclear how to properly utilize these elastic particles underground because the transport and retention are not well studied so far, especially in oil fields. This study investigates the transport and retention of novel sub-microgels in sandstone rocks, providing critical insights into their behavior in subsurface environments. A series of monodispersed sub-microgels were synthesized and characterized for size, elasticity, and swelling kinetics. Dispersing these sub-microgels in 1% KCl, the transport pressure and retention amount were determined by injecting them into sandstone rocks with known permeability and pore size distribution. We evaluated the influence of varying transport velocity, particle concentration, particle size to pore size ratio, elasticity, temperature and existence of oil phase on the transport and retention of the sub-microgels. After injection and swelling of the particles, the permeability reduction and saturation change of the rocks were investigated. The results show that the novel polymer sub-microgels can be transported easily to the in-depth of sandstone rock, with resistance factors lower than 2. Besides, the retention amount and injection pressure increase with higher oil saturation and these particles also contribute to mobilizing residual oil by wettability alteration and interfacial tension reduction. This work enhances the understanding of polymer particle transport in porous media and introduces a promising particle gel for mitigating reservoir heterogeneity in subsurface energy applications.

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References:

MS04 / 207

Continuum mechanics-based modeling of unsaturated fluid transport in poroviscoelastic food materials during conventional and microwave frying

Author: Yash Shah^{None}

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¹ *University of Illinois*

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Poroviscoelastic equations coupled with the hybrid mixture theory (HMT) based fluid transport equations were studied for conventional and microwave frying of foods. In poroviscoelastic foods, the porous structure, fluid flow paths, and mechanical behavior continuously change during frying. As frying progresses, smaller pores merge to form larger pores, cell wall thickness changes, pore sizes redistribute across a product's cross-section, and the mechanical behavior may change from viscous or elastic to viscoelastic. The material expands or shrinks depending on its nature and phenomena, such as glass transition and pore pressure. The process was modeled using hybrid mixture theory (HMT) based transport equations coupled with poroviscoelastic equations. HMT-based generalized Darcy's law can describe Fickian and non-Fickian transport in biopolymers in glassy, rubbery, and transition states. Eulerian-Lagrangian transformation was used to transform the equations from moving to stationary coordinates. The poroviscoelastic constitutive equations coupled with the momentum balance equations were used to describe the volume changes caused by positive pore pressure and shrinkage caused by elastic recovery in the material. Model validation was performed. The validated model was used to study oil uptake and textural changes in potatoes during frying. The mechanical texture changes from elastic to viscoelastic near the center and a crispier layer near the surface of material. The solution of the model provided insights into this highly dynamic process. To modify the pore pressure distribution and oil uptake, microwave frying experiments were conducted and Maxwell equations were coupled with the frying model. Using simulation results, the process parameters leading to reduced oil uptake and desirable mechanical texture were identified.

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Poster / 208

Learning Pore-scale Multi-phase Flow from Experimental Data with Graph Neural Network

Authors: Yuxuan Gu¹; Catherine Spurin²; Gege Wen¹

¹ *Imperial College London*

² *Stanford University*

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Modeling the process of multiphase flow through porous media is an essential task as it is involved in many mitigation technologies, including CO₂ geological storage, hydrogen storage, and fuel cells. To study these multiphase flow processes, scientists can utilize micro-CT scanners with synchrotron sources to image the rock pores in a nanometer-scale spatial resolution while recreating the in situ condition of gas flowing through the porous medium. State-of-the-art research facilities can now generate 3D imaging data with billions of voxels with temporal resolution in the order of seconds, creating a unique opportunity to advance our understanding of fluid flow physics.

However, despite the advancement in experimental capability to obtain high-resolution experimental data, the modeling of pore-scale multiphase flow in porous media remains very challenging. Current modeling approaches generally fall into three major classes: lattice/particle-based models, continuum models, and pore-network models. The former two approaches solve governing equations on the pore scale but are often extremely computationally expensive. Pore network models simplify

porous media into interconnected pores and throats, offering computational efficiency but usually lacking accuracy due to the complexity of the physics involved.

Machine learning-based approaches are emerging in recent pore-scale modeling studies. However, most existing studies aim to learn fluid flow physics from simulation data, which suffers from significant drawbacks. Due to the aforementioned computational challenges in pore-scale modeling, training datasets are often incapable of reflecting the accurate behavior of real-world multiphase flow. They are often simulated with highly simplified pore geometry (e.g., packed spheres) or simplified physics (e.g., negligible viscous effects and assumptions of steady-state flow). In addition, many previous approaches were designed based on convolutional neural networks (CNNs) that are optimized for grid-like structures. As a result, they struggled with the irregular geometries of complex pore structures.

In this study, we address this challenge using a graph neural network-based approach and directly learn pore-scale fluid flow using micro-CT experimental data. We used graph structure to represent irregular pore structures, where nodes represent fluid volume and edges represent fluid flow paths. Unlike traditional CNNs, the graph-based representation can handle complex geometries by passing messages only between connected nodes, ignoring nodes separated by solid rock grains. Learning the fluid flow dynamics using a GNN-based architecture leverages inductive biases to focus on local interactions between fluid and pore structures. This allows for zero-shot generalization to other boundary conditions or bigger input fields through section-based training. During inference, given an initial state, the model can autoregressively predict the evolution of the multiphase flow process over time.

Learning directly from experimental data allows us to replicate realistic flow phenomena, including those that remain beyond the reach of simulations due to incomplete understanding. Our results demonstrate that GNN can effectively capture complex fluid behaviors and generalize well across varying boundary conditions, providing a promising direction to leverage the extensive micro-CT experimental data to study pore-scale physics.

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Poster / 211

Miscible pore-scale flow and transport under variable fluid viscosity

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Miscible multiphase flow in porous media involves displacing a resident fluid by another fluid of different viscosity and density. This process arises in various applications, such as groundwater remediation, hydrogen storage, moisture and solute transport, and geological carbon sequestration,

where mixing leads to an intermediate fluid phase distinct from the original phases, thus changing the pH in a non-trivial way (1). When a less viscous fluid displaces a more viscous one, instability at the fluid–fluid interface can create pronounced “viscous fingering” patterns.

Experiments on miscible phase flow in porous media highlight the role of flow rate and heterogeneity, which also shape the emergence of fingering patterns associated with miscible phase flow. These investigations showed how a transition from homogeneous to heterogeneous pore structure leads to a uniform or finger-like invasion and how inlet pressures affect both mixing and invasion patterns, with equivalent flow rates observed at the Darcy scale. Extending this approach, the present work analyzes the impact of changing viscosity caused by mixing on the formation and suppression of fingers in a 2D porous medium. We derive solutions for the expected flow rates in a regular and irregular porous medium during the miscible displacement, as a low-viscosity fluid displaces a more viscous fluid. The derivation is based on solving the time-dependent Darcy equation over two conductivity blocks in series or parallel to capture the uniform and finger formation, respectively. This simplified solution captures well how the evolving viscosity influences hydraulic conductivity, thereby either suppressing or initiating finger formation. This solution not only captures well the experimental flux, but also the mean viscosity in the flow cell. These findings align with the effective diffusion coefficient and effective Sherwood number framework introduced previously (2).

1. A. Biran, T. Sapar, L. Abezgauz, and Y. Edery, Experimental investigation of the interplay between transverse mixing and pH reaction in porous media, *EGUsphere*, 1 (2024), publisher: Copernicus GmbH.

2. Y. Eliyahu-Yakir, L. Abezgauz, and Y. Edery, From mixing to displacement of miscible phases in porous media: The role of heterogeneity and inlet pressures, *Physical Review Fluids* 9, 084501 (2024), publisher: American Physical Society

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1. A. Biran, T. Sapar, L. Abezgauz, and Y. Edery, Experimental investigation of the interplay between transverse mixing and pH reaction in porous media, *EGUsphere*, 1 (2024), publisher: Copernicus GmbH.
2. Y. Eliyahu-Yakir, L. Abezgauz, and Y. Edery, From mixing to displacement of miscible phases in porous media: The role of heterogeneity and inlet pressures, *Physical Review Fluids* 9, 084501 (2024), publisher: American Physical Society

MS12 / 212

Investigating the Permeability Evolution of Artificial Rock During Ductile and Brittle Deformation Under Pressurized Flow

Authors: Shaimaa Sulieman¹; Shouceng Tian²; yaniv edery³

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The drilling of geothermal energy, CO₂ sequestration, and wastewater injection all involve the pressurized flow of fluids through porous rock, which can cause deformation and fracture of the material. Despite the widespread use of these industrial methods, there is a lack of experimental data on the connection between the pore pressure rise, the deformation, and permeability changes in porous structures. In this study, we developed an artificial rock material that can be deformed and fractured at low pressurized flows. By controlling the porosity, permeability, and strength of the material during the sintering process, it is possible to mimic various types of rock. The artificial rock was designed to accommodate radial flow and deformation, allowing for deformation tracking by monitoring the flux and applied pressure to calculate the permeability changes under various effective stresses. The study shows that there is a transition from dilating fracture at low effective stresses, which increased the permeability, to ductile compaction at high effective stresses, which reduced the permeability. The increased permeability due to the fracture led to hysteresis of permeability at low pressures that disappeared at high pressure due to the ductile compaction. This transition was shown to change with permeability and tensile strength and was phenomenologically captured by two models that were adjusted to this scenario.

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Poster / 214

Multi-scale Characterization of H₂ Storage in Heterogenous Carbonate Reservoirs

Author: Mohammed Al Mandhari¹

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Hydrogen energy is expected to play a significant role in the energy transition with geological storage poised to be one of the few economic options that will enable a large-scale hydrogen economy. Storage in depleted gas fields is an area of active research given the presence of legacy facilities that could be repurposed coupled with the prior knowledge of the reservoir's characteristics. Despite carbonates comprising upwards of 60% of petroleum reservoirs worldwide (Burchette, 2012), there is a critical lack of research pertaining to H₂ storage with a significant bias towards relatively homogenous sandstone reference samples and/or other gases.

The role of microporosity in geological storage remains an active research question despite the advances in pore-scale imaging. This is due to limitations arising from the low spatiotemporal resolution and field of view of CT scanners in addition to the complex nature of carbonate pore systems. Analogous research considering CO₂ storage, N₂, waterflooding and EOR indicates that microporous phases can significantly stratify flow paths into complex geometries due to their high capillary entry pressure, especially in low to intermittent fractional flows. These regions —when water-wet—can lower non-wetting phase residual saturations and boost wetting-phase relative permeabilities to aid recovery during waterflooding (Reynolds et al., 2017; Gao et al., 2019). Furthermore, the complexity

of micro-porous carbonates is further exacerbated when wettability is considered. Mixed-wet carbonates can exhibit trapping due to localized wettability alteration resulting in complex flow paths linking between micro- and macro-pores (Bultreys et al., 2016). This is coupled with contact angle hysteresis which is typically accentuated in smaller pore sizes and heterogeneous systems (e.g., van Rooijen et al., 2022).

An additional area lacking research is H₂ hysteresis across multiple cycles. Despite a majority of studies focusing on one or two cycles only, there are a few indications from microfluidic experiments that the residual trapping remains stable across multiple cycles with a strong correlation with the initial H₂ saturation; however, a consensus remains absent (Kimbrel et al., 2022; Gao et al., 2023; Lysy et al., 2023).

Following the review of opportunities and challenges associated with H₂ storage in carbonates, a research plan is proposed that aims to fill the aforementioned gaps through 4D synchrotron imaging of steady-state and cyclic unsteady-state drainage and imbibition experiments at reservoir conditions in carbonate core plugs. The samples are of low permeability and exhibit significant pore system heterogeneity. Finally, integrated field-scale reservoir simulations will be performed to assess the effect of geological structure and anisotropy. The samples display strong variations in petrophysical properties due to leaching and dissolution events, leading to the development of microporous phases with varying degrees of heterogeneity. The intricate geology of these samples renders them a strong candidate for addressing the identified research gaps in addition to supplementing the fundamental principles of imbibition phenomena in heterogeneous porous media.

Country:

United Kingdom

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MS10 / 215

Spatio-Temporal X-ray Imaging of Pickering Nanodroplets in Instability and Interaction in Porous Media

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Nanomaterials have been extensively applied for subsurface science and engineering. Generally, challenges arise due to the aggregation and deposition in the subsurface environments. The retention of the nanomaterials before the target zone reduces the amendment effectiveness and the hydraulic conductivity of the formation being treated. In this study, Pickering nanodroplet is demonstrated as an effective alternative vehicle to deliver nanomaterials in porous media with minimal retention. Two types of Pickering nanodroplets are synthesized via high-energy sonication method: one by bare iron oxide nanoparticle and the other by polymer-coated iron oxide nanoparticle. Displacement experiments were designed to evaluate the transport and retention behavior of the Pickering nanodroplets in porous media through in-situ measurements and effluent analysis. We show that the coating of the nanoparticle and ionic strength of carrier fluid for the Pickering nanodroplets determine the mode of their transport: minimal retention (I), maximum retention along the core (II), and strong retention near the inlet of the core (III). Polymer-coated nanoparticles-stabilized nanodroplets under an ionic strength of less than 0.5 M exhibit minimal retention (<0.5 wt.%) but show maximum retention (>80 wt.%) along the core under an ionic strength of 1.0 M. Significant retention (>40 wt.%) at the inlet of the core occurs for the bare nanoparticle stabilized-nanodroplets and the polymer-coated nanoparticle-stabilized nanodroplets under an ionic strength of 2.0 M. We observe the polymer detaching from the nanoparticle only in transport mode III. In transport mode II, we also report a clear-cut accumulation of the Pickering nanodroplets at the frontal end of the injection slug. These findings advance our understanding to design optimal Pickering nanodroplets for subsurface applications, with the potential to significantly enhance the effectiveness of environmental amendments in contaminated environments or other applications in oil and gas industry comprising fracture characterization or improved oil recovery.

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References:

216

On experimental and numerical study of NIR drying of LIB electrode

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Currently, convective drying is used by industry in the vast majority of battery electrode manufacturing processes. However, it is characterized by very high energy consumption and there are also limitations on the production speed. There is a demand for more efficient drying processes. Among the several technologies which are studied currently, the most promising and closest to the industrial standards is the near infrared radiation, NIR. There are a great number of experimental and numerical papers on convective drying, but NIR is still not widely studied. In this paper, we present an experimental and numerical study of electrode drying, including those with high-intensity NIR. We report several findings: (i) no vertical temperature gradient is observed in the carried experiments; (ii) NIR enables fast drying with good adhesion; (iii) no capillary limitations are observed in NIR drying of

thin electrodes; (iv) presented comparison between the experimental and numerical results, shows that the model used correctly represents the experiment; (v) we elaborate on how NIR is heating the slurry volumetrically, in contrast to the surface heating in the convective drying.

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MS21 / 217

Determination of polymer retention rate at pore size in porous media

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Polymer flooding plays a key role in enhancing oil recovery process around worldwide oil fields. Viscoelastic polymer added into water can improve sweep efficiency either by reducing mobility ratio or by lowering the degree of heterogeneity of layers [1]. It may result from factors such as the decreasing size or clogging of pore throat due to polymer retention within the reservoir rock, the elevated shear viscosity and tensile viscosity when injected fluids flows through porous media. Field calculations indicate polymer retention ranges from approximately 50 to 250 $\mu\text{g/g}$ in some reservoir [2]. Excessive polymer retention can make injection difficulty, the concentration loss deeper in reservoir, and poor oil recovery rate [3]. It is necessary to determine if polymer molecule filtrate or trap at some pore size. The objective of this work is to quantify polymer retention rate at pore size, calculate comprehensive retention rate of polymer in the core and analyze the factors on retention rate at pore size and in the core. Polymer solution filtration experiments were carried using a special uniform pore size of porous media — polycarbonate filter membrane, with pore size 0.01 μm -5.00 μm , diameter 47-48mm and thickness 9-10 μm . Partially hydrolyzed polyacrylamide (HPAM) were used as polymers with molecular weight of 14 million g/mol at 1000mg/L and 27 million g/mol at 500mg/L-1200mg/L. The polymer retention rate at pore size (Prp, %) was the percentage of polymer concentration after filtration through uniform pore size of porous media and before filtration, and polymer concentration was measured through a range of uniform porous media by starch-cadmium iodide method. The comprehensive retention rate of polymer in the core (Prc, %) was calculated by combining the pore size distribution with polymer retention rate varying from pore size. The results show that there is obvious correlation between retention rate of HPAM at pore size and Rtp, which is the ratio of pore throat radius (Rt) to polymer hydrodynamic radius (Rp) and is used to characterize the relative size of polymer molecule and pore throat (Fig1.). It is found that when $Rtp \leq 0.5$, retention rate can reach about 80%; When $0.5 < Rtp \leq 1.2$, 20%-80% of the retention occurs, and retention rate is less than 20% when $Rtp > 1.2$. The comprehensive retention rate increases significantly with the decrease of permeability. When the permeability decreases from 1000mD to 50mD, Prc increases from 30% to 60% (Fig2.). The higher the molecular weight, the larger the concentration and the higher the retention rate. The comprehensive retention rate of polymer in the core can predict the clogging degree of polymer and the retention rate at pore size can be further used to determine the distribution of polymer trapped in reservoir.

Country:

China

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

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MS18 / 218

Combining Aquifer Tests, Dye Tracing, and Discrete Fracture Network Modeling for Characterizing Solute Transport in a Fractured Aquifer

Author: Phillippe Lima¹**Co-authors:** Anthony Runkel²; Jana Kramer¹; Peter Kang¹; Qifei Niu³; Seonkyoo Yoon⁴; Warren Barrash³¹ *University of Minnesota*² *Minnesota Geological Survey*³ *Boise State University*⁴ *University of Florida*

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Fractured aquifers impose challenges in predicting solute transport as the complex connectivity within discrete fracture networks, mass exchange between rock matrix and fractures and heterogeneous rock permeability should be considered. This research presents a holistic approach to characterize hydrogeologic features of fractured aquifers and to establish a predictive model for flow and transport processes. We focus on a field site located in the University of Minnesota, Twin Cities campus, which has been developed as a research and teaching facility for the purpose of improving our ability to predict groundwater flow and solute transport in fractured rock aquifers.

Tracer tests conducted at the site revealed a strong tailing with power law slopes of 1.1 and 1.29. Aquifer tests, borehole logging, Discrete Fracture Network (DFN) modeling, and Electrical Resistivity Tomography (ERT) were conducted to improve the subsurface characterization and assess the role of matrix and fractures on producing the anomalous solute transport observed in the breakthrough curves.

Ten injection tests were performed using three Multi-Level Hydraulic Packer and Port Systems (MHPS) that isolated the main Bedding Parallel Parting fracture (BPP) and measured water level responses with pressure transducers and Fiber-Optics pressure transducers. Subsurface parameters

were estimated by using various pumping test analytical solutions for porous and fractured media.

These field data, and fracture statistics obtained from outcrops, were incorporated into a three dimensional Upscaled Discrete Fracture Matrix (UDFM) model to simulate flow and transport processes at the field site to reproduce the tracer tests. Achieving predictability, especially in late-time regimes, simulation results with sensitivity analysis suggests that high matrix permeability underpins the strong tailing.

Ongoing DFN simulation aims to assess the role of fractures on the anomalous solute transport and a Hydraulic Tomography inversion is planned to evaluate the connectivity and pathways across the site. Preliminary ERT results showed promise approach for tracking the injected water displacement and highlighting the water pathways in the fractured system.

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United States

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MS25 / 219

A scaling law for reaction-induced fracturing during mineral carbonation and hydration

Author: Masaoki Uno¹

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Mineral carbonation and hydration involve a large solid volume increase of tens of percent and may result in clogging of pores in the rocks and inhibit further reaction. On the other hand, natural observation of carbonated or hydrated peridotite and serpentinite suggests that the volume increase of the reactions can fracture rocks, enhance fluid flow, and promote further reactions [1,2]. Such reaction-induced fracturing has been considered as a key process promoting subsurface mineral carbonation, however, up to now, the majority of laboratory carbonation experiments result in pore clogging and have not reproduced macroscopic fracturing.

Here we show a clear experimental example of macroscopic reaction-induced fracturing caused by carbonation of brucite-rich serpentinite. During the reaction with CO₂-saturated water, the brucite selectively dissolves from the sample surface, with minor magnesite precipitation on the surface and no fracturing. In contrast, the reaction with NaHCO₃ solution shows that brucite selectively

dissolves at the reaction fronts, and magnesite precipitates within the pre-existing micro-cracks, causing macroscopic fracturing of the sample, which promotes further carbonation in the sample interior. These contrasting mechanical responses during carbonation in our experiments, as well as differences in the previous laboratory experiments and field-scale carbonation, would be explained by the competition between the rates of carbonate precipitation and rates of solute transport, and may provide clues for the acceleration of anthropogenic mineral carbonation.

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Japan

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References:

1: Kelemen and Matter 2008 PNAS, 105, 17295–17300. 2: Uno et al. 2022 PNAS, 119, e2110776118.

223

Hybrid data-driven model for seawater intrusion in coastal aquifers

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Seawater intrusion poses a significant threat to aquifer resources in coastal areas, primarily driven by climate change and overexploitation. Due to uncertainties associated with hydrogeology and climate predictions, physical modeling can often be cost-prohibitive or inaccessible. To address this challenge, we propose a data-driven method to analyze and predict the behavior of the phreatic aquifer in the Emilia-Romagna region of Italy. We have developed a statistical modeling tool called DRONE, which employs a non-stationary Gaussian Process (GP) [1,2] for each piezometer well. The non-stationary kernel function we use provides an advantage in estimating local trends across different cross-sections. This model effectively describes and predicts seawater intrusion in both spatial and temporal dimensions. To render the mean function non-stationary, we incorporate climate data, such as precipitation and temperature, to assess the impact of climate change. We apply the non-stationary GP model to combine predictions from each well, creating a comprehensive forecasting map for the regional coastline. This map illustrates the seasonal distribution of salinity and aids in risk assessment. To improve predictive robustness, we introduce a physically informed structure for our data-driven model. Since full-scale physical simulation is often computationally intensive, our physical model is either an analytical or a low-fidelity numerical scheme. We then treat the GP model as a source of model error, allowing us to assimilate the physical model with observational data. This physically informed framework enables long-term predictions and provides a physical explanation that supports the design of Managed Aquifer Recharge (MAR) systems. Additionally, the DRONE model can be applied to predict various water quality components. This research is part of the EU-funded MAR2PROTECT project (GA n. 101082048, HORIZON programme), which aims to develop innovative MAR strategies to combat groundwater contamination.

Country:

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MS03 / 225

Damage induced by salt crystallization in heterogeneous porous media in the context of the erosion of the French Basque Coast and the damage of protective buildings

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Coastal erosion is a growing concern for many coastal regions worldwide, and salt weathering has been identified as a contributing factor to this phenomenon. This research focuses on the ongoing erosion of the French Basque Country coastline, particularly between the connecting sections of Saint-Jean-de-Luz and Hendaye which are characterized by Santonian flysch rock cliffs.

The objective of the global project is to investigate the role of salt weathering and its impact in the mechanical weakening of both the tight and low-porosity flysch rocks with rhythmic alternations of heterogeneity and the concrete material used for the protective blocs of the Artha dam located in Saint-Jean-de-Luz. Particularly, this study focuses on the gathering of reliable and fine experimental data allowing the calibration and the validation of predictive numerical tools developed besides.

For this purpose, a novel accelerated salt weathering protocol has been developed, involving the continuous partial immersion of test samples in a 3 molal concentration of sodium sulfate solution at a controlled temperature of 34 °C, while maintaining room temperature at 20 °C. Non-destructive acquisition techniques, including acoustic emission analysis and time-lapse photography or quasi-simultaneous neutron and x-ray tomography (Institut Laue-Langevin) –coupled with digital image correlation –were employed to gather reliable experimental data for validating the weathering protocol and for further numerical analysis. The effectiveness of the protocol was confirmed through numerous tests conducted on the two targeted materials (flysch rocks and Artha dam concrete) but also on Vosges sandstones, which are less heterogeneous and widely studied in the literature.

Central to this study, the unique application of quasi-simultaneous neutron and x-ray imaging provided a comprehensive understanding of the role of salt crystallization in damaging porous rock materials with encouraging experimental data acquired to enable the observation and quantification of fracture formation and hydrated salt content in the samples. The results gathered indicate that salt crystallization is a crucial factor in the observed damage of flysch rock, Vosges sandstone, and concrete samples, with heterogeneity playing a significant role in the deformation and failure.

The findings of this study contribute valuable insights into the phenomenon of crystallization-induced damage by salt, which has practical applications in building engineering, materials science, and environmental science. The collected experimental database, especially on Vosges Sandstone, can be directly used for numerical model calibration and validation.

Acknowledgements:

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Newpores. H. Derluyn acknowledges the support from the ERC Starting Grant PRD-Trigger (grant agreement N° 850853). The authors gratefully acknowledge Alessandro Tengattini and Lukas Helfen for their help and support during the experimental tests carried out at the D50 beamline of the Institut Laue-Langevin (Grenoble, France).

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References:

MS02 / 226

Synchrotron and Conventional Analyses of Soil Pore Properties Influencing Cohesion in Coastal Tablelands Soils

Author: Talita Rosas Ferreira¹

Co-authors: Brivaldo G. de Almeida²; Jaedson C. A. Mota³; José C. de Araújo Filho⁴; Francisco M. C. da Silva¹; Tiago O. Ferreira⁵; Larissa M. Moreno¹; Luiz F. Pires⁶; Karina M. V. C. Polizeli⁷; Dean Hesterberg⁸

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Many soils in the Coastal Tablelands of Brazil have limitations in their physical quality because of subsurface cohesive horizons [1]. The consistency of cohesive soil horizons is hard to extremely hard when dry, restricting root development, while its structure slakes under high water content, reducing the support of plants and drainage [2,3]. Often, sand constitutes 70% to 80% of cohesive soil horizons, and thus fine illuvial clay is considered to have an important role in the formation of cohesion by promoting pore obstruction and decreasing total porosity [1,4]. Soil cohesion is assessed by penetration resistance (PR) measurements, often exceeding 2 MPa at field capacity, a threshold that can restrict root growth [5].

The CNPEM-Embrapa Cohesive Soils Program launched in March 2024 aims to determine mechanisms causing cohesion in subsurface horizons of soils found in ~100,000 km² of the Tablelands region of Brazil. The program analyzes synchrotron and conventional data from samples of three soil profiles with cohesive horizons, designated as profiles P1 and P2 in Pernambuco and C1 in Ceará. The present study is part of this collaborative program and aims at determining contributing conditions for the cohesion mechanism to be effective. For example, we hypothesized that: 1) cohesion increases with decreasing total porosity due to a lower proportion of macropores between sand grains and an increase in micropores within the clay infilling between sand grains; and 2) cohesion

increases with decreasing connectivity of pores in the clayey fabric.

To investigate these hypotheses, 19 samples (seven from P1, six from P2, and six from C1) were scanned by X-ray computed tomography at the MOGNO beamline of the Sirius synchrotron in Brazil [6], yielding 3D images with pixel size of 3.4 μm . Image based total porosity, and fractions, connectivity, and tortuosity of macro ($>50\text{ }\mu\text{m}$ diameter), meso (15-50 μm), and micropores (3-15 μm) were determined. In addition, laboratory and field PR were measured in samples from the same profile depths.

Cohesion increased significantly ($p < 0.01$) with decreasing total porosity for the combined data from profiles P1 and P2, and more specifically, cohesion increased significantly ($p < 0.01$) with increasing proportion of micropores and decreasing proportion of macropores. Although not statistically significant ($p > 0.05$), data from profile C1 suggested the same trends. More generally, PR showed significant ($p < 0.01$) inverse linear relationships with connectivity of macropores for profiles P1 and C1 (same trend for P2, not significant), and with connectivity of mesopores for profiles P1 and P2. However, although micropores should be more prevalent within the clay ($<2\text{-}\mu\text{m}$ particle) fabric, simple linear regression models between PR and connectivity of micropores were not significant ($p > 0.05$). No trend between PR and micropore connectivity was shown by the lab data for profile C1. The results support hypothesis 1 and refute hypothesis 2. Although the present study does not explain the cohesion mechanism, it contributes to understanding porosity conditions in the cohesive horizons.

Country:

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Water & Porous Media Focused Abstracts:

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References:

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Effect of Adsorption Layer on Gas Flow Capacity in Shale Micro-Nano Pores

Author: Xianggang Duan¹

Co-authors: Zhiming Hu¹; Yingying Xu¹; Jin Chang¹

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Shale gas reservoirs are characterized by complex micro- and nano-scale pore structures, where gas exists as free gas, adsorbed gas, and dissolved gas. The adsorption layer, primarily forming on organic matter and clay mineral surfaces, significantly influences gas flow dynamics. When the radius

of the gas flow channel approaches the molecular free path, the wall interface layer becomes critical. In nanoscale pores, methane adsorption layers and water films reduce effective pore diameters, affecting gas molecule migration and altering flow regimes.

This study measured pore size distributions in shale samples using mercury injection and gas adsorption methods and tested gas flow capability with a steady-state flow simulation device. Results revealed that adsorption layers, with a thickness under 1 nm as determined by potential energy functions, impact flow through Knudsen diffusion and slippage effects. These mechanisms, both caused by gas-wall interactions, should not be simultaneously considered in flow calculations. An apparent permeability model incorporating boundary layer effects was developed to describe gas flow in shale pores accurately.

Flow experiments validated the model, demonstrating its ability to fit experimental and production data. This practical model supports production modeling and recovery predictions in shale gas reservoirs. These findings enhance understanding of adsorption layer dynamics, providing a basis for optimizing gas recovery and reservoir management in Shale gas reservoirs.

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References:

MS13 / 228

A novel DFT for associating fluids confined in nanopores and its application to water

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A new free-energy functional is first proposed for inhomogeneous associating fluids. The general formulation of Wertheim's thermodynamic perturbation theory is considered as the starting point of the derivation. We apply the hypotheses of the statistical associating fluid theory (SAFT) in the classical density functional theory (DFT) framework to obtain a tractable expression of the free-energy functional for inhomogeneous associating fluids. Specific weighted functions are introduced in our framework to describe association interactions for a fluid under confinement. These weighted functions have a mathematical structure similar to the weighted densities of the fundamental-measure theory (i.e. they can be expressed as convolution products) such that they can be efficiently evaluated with Fourier transforms in a 3D space. The resulting free-energy functional can be employed to determine the microscopic structure of inhomogeneous associating fluids in arbitrary 3D geometry. The new model is first compared with Monte Carlo simulations and previous DFT versions for an associating hard-sphere fluid against a planar hard wall in order to check its consistency in a 1D case. As an example of application in a 3D configuration, we then investigate the extreme confinement of an associating hard-sphere fluid inside an anisotropic open cavity with a shape that mimics a simplified model of zeolite. Both the density distribution and the corresponding molecular bonding profile are given, revealing complementary information to understand the structure of the associating fluid inside the cavity network. The impact of the degree of association on the preferential positions of the molecules inside the cavity is investigated as well as the competition between association and steric effect on adsorption.

Well-known for its ability to form oriented interactions that are hydrogen bonds, water belongs to the class of associative fluids. A SAFT-based DFT water model has been developed by using the new

association functional as a perturbation of a Mie-monomer. We first employed the new model to investigate the behavior of water confined in slit-like nanopores made of graphitic surfaces for several configurations and thermodynamics conditions. The graphite - water - graphite system has already been studied with other SAFT-based DFT formulation such that it can be used to see the impact of the different SAFT-DFT frameworks on the density distributions and thermodynamics properties. When crystallization occurs in a pore, the interactions between the crystal and the skeleton have led to the concept of “crystallization pressure”. It has been supposed that the interaction should be mediated by the presence of a thin water fluid film located in between them. Hence, a ice - water - graphite system has then been studied with the new SAFT-based DFT formulation by considering the ice crystal as an external potential applied to the inhomogeneous water film. In this way, we could obtain the equilibrium distribution of water molecules confined into a slit-like nanopore consisting of an ice crystal on one side and a graphitic surface on the other side (see figure 1). Several configurations and thermodynamics conditions have been explored and the pressure of this inhomogeneous film has been analyzed.

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References:

MS06-A / 229

The impact of small-scale heterogeneities on residual trapping: case study from the Otway CO₂ storage site

Authors: Catherine Spurin¹; Mitch Allison²

Co-authors: Catherine Callas ; David Bason ²; Sally Benson ¹

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The injection of CO₂ into subsurface reservoirs provides a long-term solution for anthropogenic emissions. However, rapid plume migration, not predicted in typical reservoir simulations have been observed at CO₂ storage projects such as the Sleipner project. Recent work has shown that small-scale heterogeneities, not currently included in reservoir models, can manifest as rapid field-scale plume migration [1]. These small-scale heterogeneities will also influence trapping, so it is important to understand their impact on CO₂ storage projects.

In this work, we explore the impact of small-scale heterogeneities on the distribution and trapping of CO₂ in core-scale samples (5cm diameter) from the Otway storage site in Australia. We perform steady-state CO₂ injection into samples from the site, and image the CO₂ distribution using a medical CT scanner. We measure the relative permeability and trapping efficiency for the samples.

A wide range of heterogeneities were observed, shown in Figure 1. We observed fine layers (Figure 1a), thicker layers (Figure 1b) and more complex patterns of heterogeneity (Figure 1c) over a narrow interval of 5m. As can be observed in Figure 1, these different heterogeneities lead to a wide range

of CO₂ distributions, as well as the subsequent trapping. The scale over which these heterogeneities impact the flow and trapping of CO₂ is much smaller than the grid sizes than in typical reservoir models. We explore how the small-scale heterogeneities control the flow of CO₂ in the subsurface, and how they cannot be ignored at the field scale. These results form the Special Core Analysis (SCAL), whose inputs are being used to model the injection of 10,000 tons of CO₂ in the Otway basin.

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Water & Porous Media Focused Abstracts:

References:

MS17 / 230

Local thermal non-equilibrium processes in porous media: Comparison of different models from the pore- to the REV-scale

Authors: Anna Mareike Kostecky¹; Rainer Helmig²; Ivar Stefansson³; Carina Bringedal⁴; Tufan Ghosh⁵; Helge Dahle³

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² *University of Stuttgart*

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Local thermal equilibrium, meaning an instantaneous heat transfer between different phases, is often assumed when modeling heat transfer in porous media systems. However, for some technical applications as well as environmental systems, such as self-pumping transpiration cooling [2], fuel cells [4] and geothermal systems [3], heat exchange processes between the different phases may be of great importance e.g. due to large temperature gradients or large differences in thermal properties of the respective phases. Therefore, when modelling those processes, local thermal non-equilibrium (LTNE) processes should be considered to evaluate the validity of the instantaneous heat transfer assumption.

In our presentation, we show a comparative study for conduction as well as conduction and convection processes between three different LTNE-models focusing on the influence of the interface between a solid and a single fluid phase. On the one hand, the pore-scale geometry including the solid-fluid interface will be resolved by the grid and the respective equations are solved for each phase and coupled through interface conditions. On the other hand, two additional models leading to averaged physical properties, such as the temperature, are taken into consideration. The dual network model ([5]) hereby takes the pore geometry still into account by approximating it with ideal shapes, while a model on the Representative Elementary Volume (REV) scale ([6]) accounts for

the pore-scale geometry through averaged quantities. For the latter, different effective conductivity approaches (e.g. obtained through homogenization [1]) are considered, indicating the importance of the respective choice. Additionally, we will provide a short outlook on recent ongoing model developments regarding interfacial heat transfer, including a coupled porous-media free-flow model for local thermal non-equilibrium processes.

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References:

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MS25 / 231

Direct visualization of coupled mineral dissolution and precipitation to predict pore-clogging dynamics

Authors: Jieun Kim¹; Jinil Park¹; Yeonuk Yu¹; Seunghyeok Han¹; Sudong Park¹; Weonshik Han²; Peter K. Kang³; Rhokyun Kwak¹

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Mineral dissolution and precipitation play a critical role in geofluid processes such as CO₂ mineralization, subsurface H₂ storage, and in-situ leaching. Despite their importance, the coupled dynamics of dissolution and precipitation underexplored, as most studies have examined them independently. In this study, we investigate the interplay between mineral dissolution and precipitation, focusing on their influence on pore-clogging dynamics. Using a microfluidic device with two embedded NaCl crystals and a straight channel, we directly visualize the simultaneous dissolution of NaCl and precipitation of AgCl as a mixture of AgNO₃ solution and ethanol flows through the channel. By adjusting

the concentrations of ethanol and AgNO_3 , we control the dissolution and precipitation rates, enabling systematic analysis of their effects. Through the pore-scale visualization, we reveal distinct dissolution and precipitation patterns under varying flow velocities and dissolution/precipitation rates, leading to different pore-clogging behaviors. Predictably, conditions with fast flow, rapid dissolution, and slow precipitation minimize clogging, while the opposite conditions exacerbate it. Interestingly, at intermediate conditions—where dissolution and precipitation rates are comparable—we observe dynamic transitions in pore-clogging over time. During the initial stage, at a given flow rate, mild clogging occurs in the channel between NaCl crystals, accompanied by subtle pressure fluctuations as accumulated precipitates are periodically flushed out. Over time, as the channel widens due to NaCl dissolution, precipitates accumulate near the NaCl crystals, leaving the center of the channel empty. However, as the channel widens further, the local flow velocity continues to decrease, allowing more precipitates to remain within the channel. Eventually, these precipitates tightly clog the outlet, leading to a rapid pressure increase. Through scaling analysis of dissolution and precipitation boundary layers in relation to flow rates and dissolution/precipitation rates, we identify the critical conditions for tight pore clogging. To the best of our knowledge, this study is the first to quantify and elucidate the coupled effects of mineral dissolution and precipitation on pore-clogging dynamics. Our findings offer critical insights into mineralization processes and pore-clogging prediction, with practical implications for subsurface resource management and geofluid engineering.

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MS26 / 232

Impact of Ostwald ripening on the stability of capillary-trapped CO_2 : a retrospective

Authors: Charlotte Garing¹; Sally Benson²

¹ *University of Georgia*

² *Stanford University*

Corresponding Authors: smbenson@stanford.edu, charlotte.garing@uga.edu

Capillary trapping is a key mechanism that increases CO_2 storage security by immobilizing a substantial fraction of the injected CO_2 in the pores of the reservoir formation. The long-term stability of capillary-trapped CO_2 is desirable, as remobilization of the trapped phase impacts the extent and rate of CO_2 plume migration and CO_2 dissolution and mineralization. Redistribution of the trapped CO_2 phase may happen due to mass transfer driven by differences in capillary pressure between trapped CO_2 ganglia, a process called Ostwald ripening.

This presentation details the early research dedicated to Ostwald ripening in porous media with application to geologic carbon storage, led by Sally Benson's group. This includes experimental investigations using time-lapse x-ray microtomography imaging and the first pore-scale and continuum-scale modeling work. The talk also briefly reviews studies that this body of work has inspired in recent years and summarizes the main findings regarding the role of Ostwald ripening on the stability of capillary trapping.

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United States

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Poster / 234

Biogeochemical Conditions Impacting Hydrogen Storage in Gypsum-Anhydrite-Rich Salt Caverns

Author: Julia Barkelew¹¹ *The University of Texas at Austin***Corresponding Author:** julia.barkelew@utexas.edu

The widespread deployment of wind and solar energy across the United States, along with the increasing use of electrolyzers to convert excess off-peak energy into pure hydrogen from freshwater, offers a promising pathway to reduce the nation's reliance on carbon-based fossil fuels and facilitate a steady transition to reliable renewable energy sources. Hydrogen is an attractive energy carrier because of its high energy density, natural abundance, and carbon dioxide-free oxidation process. The produced hydrogen can then be injected into solution-mined cavities within salt formations, offering a large-scale, long-term storage solution to supplement energy production during periods of low wind and solar output.

Gypsum-anhydrite-rich formations interbedded with halite are of particular interest for hydrogen storage due to their self-healing properties, large deformation capacity, and geographical overlap with existing renewable energy hubs in the US. However, significant knowledge gaps still persist regarding the feasibility of long-term hydrogen storage in salt caverns, primarily due to hydrogen's high reactivity and the complex biogeochemical conditions within these caverns. Sulfate-reducing bacteria, anaerobic halophiles commonly found in salt caverns, are of particular concern due to their ability to utilize dissolved sulfate minerals as electron acceptors and hydrogen as an electron donor, reducing sulfate to hydrogen sulfide—a highly corrosive and toxic byproduct. This reaction can lead to the leakage of hydrogen sulfide through pore fractures into overlying potable groundwater aquifers, contaminating drinking water sources and threatening public health. Additionally, this reaction depletes stored hydrogen and alters brine chemistry, posing significant risks to the efficiency and safety of underground hydrogen storage systems.

Understanding the role of sulfate reducing bacteria in hydrogen consumption and their potential adverse effects on overlying potable water aquifers is imperative as hydrogen storage in salt caverns becomes a widely adopted energy storage solution. By utilizing a biogeochemical modeling software, CrunchFlow, the impacts of hydrogen leaks into shallow aquifers above storage sites will be analyzed, offering relevant information required to optimize underground storage system efficiency, performance, and scalability.

The model will simulate hydrogen consumption over time in batch experiments, taking into account factors such as electron acceptors, pH, and ionic strength. The model will also include mineral speciation and gas-water-rock partitioning reactions at equilibrium. The simulation will be modeled as a closed system, with both a liquid phase for the brine present in cavities and a headspace containing gaseous components such as hydrogen and nitrogen, assuming ideal behavior for gas partitioning. Key factors influencing sulfate reduction, such as pH, partial pressure, and brine salinity, will be systematically varied to assess their impact on sulfate reduction reaction kinetics.

The modeling results are expected to identify parameters governing hydrogen consumption over time in batch experiments and increase reaction kinetic parameter accuracy for hydrogen consumption calculations associated with other microbial communities expected to be found in halite storage

reservoirs.

Ultimately, this research aims to identify environmental conditions that minimize microbial-driven hydrogen consumption in underground halite reservoirs, supporting the large-scale deployment of hydrogen storage and advancing the transition to a more sustainable energy future.

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MS06-A / 235

Two-phase flow and reactivity: an hybrid-scale approach

Author: Cyprien Soullaine¹

¹ *CNRS Orléans*

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In this work, we present advanced numerical models to simulate two-phase flow in reactive environments across multiple scales of interest. The model seamlessly integrates continuum-scale and pore-scale reactive transport within a unified framework using the same set of partial differential equations. It extends the Darcy-Brinkman-Stokes formulation to two-phase flow, enabling a comprehensive description of flow dynamics in both resolved and unresolved regions.

In resolved regions, the fluid-fluid interface is dynamically tracked using a volume-of-fluid approach, while the fluid-solid interface evolves in response to chemical reactions. In unresolved regions, two-phase flow is modeled using effective properties, including relative permeabilities and capillary pressure. This dual-scale approach ensures consistency and adaptability across varying levels of resolution.

The capabilities of the model are demonstrated through simulations of mineral dissolution and the subsequent gas exsolution processes, capturing critical reactive transport phenomena at both the pore-scale and continuum-scale. These results underscore the model's potential for advancing our understanding of coupled flow and reactive transport processes in complex environments.

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Poster / 237

DuMux –an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling

Authors: Anna Mareike Kosteletzky¹; Timo Koch²; DuMux developer team^{None}

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² *University of Oslo*

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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 3.10, Spring 2025) 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 “Water” 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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Water & Porous Media Focused Abstracts:

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References:

Timo Koch et al. “DuMux 3 –an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling”. In: *Computers Mathematics with Applications* 81 (2021). Development and Application of Open-source Software for Problems with Numerical PDEs, pp. 423–443. issn: 0898-1221. doi: <https://doi.org/10.1016/j.camwa.2020.02.012>.

MS26 / 240

Thermodynamics of Ganglia in 2D Porous Media

Author: Chuanxi Wang¹

Co-author: Ke Xu¹

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Ganglia (bubbles, or droplets) are widespread in porous media of various industrial applications such as geological carbon dioxide storage. 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 (Armstrong et al., 2018; Wang et al., 2021), quantitative description of ganglia in heterogeneous media remains a challenge (Huang et al., 2023; Li et al., 2020).

In this study, we develop a pore-scale algorithm for determining the morphologies and thermodynamic properties of hydrostatic ganglia in heterogeneous porous media. By tracking cycles of quasi-static growth and shrinkage of a ganglion, we resolve the evolution of P_c (Figure 1a). During growth, the ganglion invades pore by pore, with the throat length as the primary length scale that controls P_c . In contrast, during shrinkage, the ganglion collapses inward as a whole, exhibiting multiple scales of P_c at different stages. Additionally, we identify a critical ganglion volume, V_{crit} (black dashed lines in Figure 1a). Beyond V_{crit} , the P_c of a growing ganglion consistently exceeds that of a shrinking ganglion with the same volume, indicating that the ripening of such ganglia is not kinetically favorable. While we provided a thermodynamic critical volume for ganglia ripening in InterPore2024, this work introduces a kinetic critical volume.

Furthermore, we compare behaviors of growing and shrinking ganglion in different porous media with varying degrees of heterogeneity (Figure 1b). In both cases, the ganglion seeks the region of lowest energy, corresponding to areas with the smallest local pore-throat ratio in the porous medium. The greater the heterogeneity, the later the transition of the F - V relationship from sub-linear to linear (as referenced in InterPore2024), and the lower the final specific surface area. Although there are both narrow and wide throats in a heterogeneous porous medium, the behavior of the ganglion is consistently governed by the narrower throats.

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 porous media. We believe that this work helps better understand the behaviors of the dispersed phase in porous media.

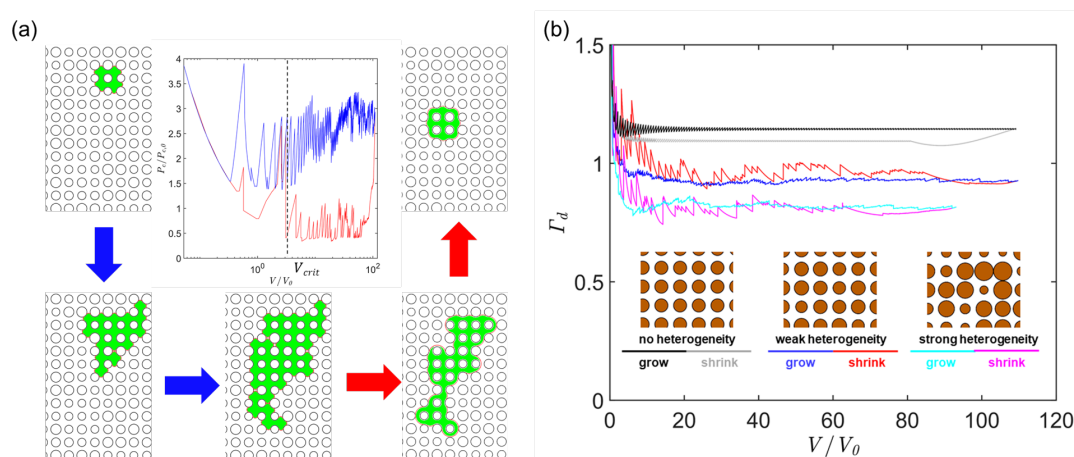


Figure 1: (a) Snapshots of ganglion growth and shrinkage in heterogeneous porous media. The relation between capillary pressure and ganglion volume. (b) Effect of heterogeneity on specific surface area.

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References:

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MS17 / 241

Experimental and computational study of solidification of flow in a Hele-Shaw cell

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The warming climate is inducing changes in hydrological processes in the cryosphere that are not well understood. In this context, the proposed work seeks to advance our understanding of the pore-scale physics of fluid flow through subfreezing porous material such as snow, firn and permafrost.

Such flow involves the complex interplay amongst interfacial flow (e.g. air-water), phase change (e.g. freezing/melting), and thermal transfer between liquid-liquid or liquid-solid phase boundaries, giving rise to a myriad of non-equilibrium phenomena from pore to field scales.

Here, we couple novel laboratory experiments and high-resolution simulations to characterize this type of flow in the simplified configuration of a Hele-Shaw cell. To conduct the experiments, we radially inject water at 0°C and a constant flow rate into a Hele-Shaw cell that is being cooled by an aluminum plate placed in a freezer at -80°C for 24 hours to induce solidification in the cell. We systematically vary the initial gap thickness and flow rate to observe changes in the solidification dynamics and flow.

Next, we simulate the experiment with a continuum model, where we couple the single-phase Hele-Shaw flow equations with a gap-averaged formulation of heat transfer and phase change that accounts for reduction in gap thickness due to freezing. We perform numerical simulations of the model in both 1D and 2D and study the role of injection rate, initial thermal conditions and initial gap thickness on the temperature evolution and pattern formation of the flow. Finally, we provide preliminary results that validate the model with experiments.

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MS25 / 242

Pore Network Modeling of Coupled Mineral Dissolution and Precipitation in Fractured Porous Media

Author: Agnieszka Budek¹

Co-authors: Piotr Szymczak²; Peter Kang¹

¹ *Department of Earth and Environmental Sciences, University of Minnesota – Twin Cities, Minneapolis, USA*

² *Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland*

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Understanding the interplay between mineral dissolution and precipitation in fractured porous media is crucial for advancing carbon mineralization processes. Fractures are often expected to act as highways for supplying CO₂-charged water, while the matrix is anticipated to serve as a storage space. However, how the interplay between mineral dissolution and precipitation controls mineralization in fractured porous media remains unclear. In this study, we develop a pore network model to investigate coupled dissolution-precipitation reactions within a fracture-matrix system. The dynamic interaction of flow, transport, reactions, and geometry evolution in such systems gives rise to a variety of pattern formation regimes: from rapid fracture passivation to intense side branching and nearly homogeneous transformation of the rock matrix into the product phase. In addition to exploring these regimes, we aim to determine the conditions that optimize precipitate deposition—achieving significant mineralization without causing severe clogging.

Our results reveal that spatial separation between dissolution and precipitation can lead to fracture passivation under specific conditions (see Fig. 1), while rapid precipitation and “in-situ” deposition of secondary material may result in a uniform transformation of the rock matrix (see Fig. 2). Moreover, partial clogging within fractures induces side branching, maximizing precipitation and enabling minerals to deposit deeper into the system (see Fig. 3).

Further, we explore the impact of operationally controllable parameters, such as flow (injection) rate and inlet reactant concentration. The flow rate determines the length and density of side branches, while the inlet concentration governs the rate of fracture passivation. This work provides valuable insights into optimizing carbon mineralization in fractured porous systems, enhancing our understanding of the dynamic processes underlying mineral dissolution, precipitation, and system evolution.

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Poster / 243

Mathematical Modeling of Carbonated Waterflooding: Analytical Solutions for Low-Carbon Enhanced Oil Recovery

Author: Saulo Aguiar¹

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The transition to a low-carbon economy emphasizes innovations that reduce greenhouse gas emissions while enhancing energy and production efficiency. Among the strategies adopted by oil and gas (O&G) companies is carbonated waterflooding, a method of enhanced oil recovery (EOR-CO₂) that involves injecting carbonated water into reservoirs. This technique not only improves oil recovery but also contributes to carbon sequestration by storing CO₂ in subsurface formations.

Although carbonated waterflooding has been studied since the mid-20th century, the process introduces complex interactions between CO₂, reservoir rocks, and fluids (oil and water) that require detailed evaluation. Key mechanisms include oil swelling, viscosity reduction, miscibility effects, and geochemical interactions. A comprehensive understanding of these processes is critical for optimizing recovery and aligning with low-carbon economy objectives.

This work presents an analytical model for carbonated waterflooding in porous media saturated with oil and water. The study evaluates the interactions between CO₂, reservoir rocks, and reservoir fluids, focusing on a three-component system (oil, water, and CO₂) in two phases (aqueous and oleic). The model is derived using mass conservation equations in a one-dimensional, homogeneous, incompressible, and isothermal system. Simplifying assumptions include constant porosity and permeability, negligible dispersion, capillary, and gravitational effects, and the absence of chemical reactions. However, interphase mass transfer between oil, water, and CO₂ is incorporated, along with CO₂ adsorption onto the solid phase.

The findings offer insights into the dynamics of carbonated waterflooding and its potential to enhance oil recovery while contributing to carbon sequestration goals.

By providing an analytical framework, this work advances the understanding of carbonated water-flooding as an EOR technique, offering a basis for optimizing field applications and supporting the development of sustainable oil recovery strategies aligned with global low-carbon goals.

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Poster / 244

Mechanical Performance of Accelerated Carbonated Concrete

Authors: Geng Niu¹; Kaina Rodrigues Vieira¹; SONIYA Tiwari^{None}; Qinyi Tian^{None}; Laura Dalton¹

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As the global demand to limit the heating of the planet to 1.5 to 2.0 °C by 2050 becomes increasingly urgent, the CO₂ mineralization reactions of Portland cement concrete (i.e., carbonation) have emerged as a large-scale CO₂ capture and sequestration solution. Portland cement, the primary ingredient in concrete and the second most widely used material after water, has the potential to mineralize CO₂ into stable calcium (and magnesium) carbonates. While carbonation is reported to refine pore structure and enhance its mechanical performance, its effect on the relationship among deviatoric stress, material deformation, and failure mechanisms of the concrete remains insufficiently understood. In this study, we investigate the coupled effects of accelerated carbonation on the mechanical performance of concrete using both an Environmental Triaxial Automated System (ETAS) and a TESCAN UniTOM XL X-ray micro-computed tomography (X-CT) scanner.

To analyze mechanical performance, ETAS (triaxial tests) were conducted, and results were used to construct P-Q stress state diagrams to reveal the relationship between mean normal and deviatoric stresses. Further analysis using the Mohr-Coulomb failure criterion was used to quantify critical parameters, providing detailed insights into the failure mechanisms and stress behavior of carbonated concrete. X-CT was used to both monitor the evolution of carbonation depth before ETAS testing and failure cracks on the same samples after ETAS. This non-destructive, high-resolution technique facilitated continuous monitoring of the spatial and temporal progression of carbonation, including the pore structure alterations and the distribution of carbonation products. Additionally, X-CT was used to capture and analyze the interplay between carbonation and fracture propagation, offering a comprehensive understanding of these coupled processes. This research advances the fundamental understanding of accelerated carbonation in concrete in support of the transition toward carbon-neutral solutions in the built environment.

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245

Pore-Scale Insights into Water Transport in Clay: Modeling with Classical Density Functional Theory

Author: Abdullah Cihan¹

Co-author: Pramod Bhuvankar¹

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Water transport in nanoporous media is essential for many scientific and engineering applications. However, the phase behavior and transport properties of water in nanoconfined pore spaces are not yet fully understood. In the context of geoscience applications, discussions have long persisted about whether flow through fine-grained porous media, such as clay, deviates from Darcy's law. Literature suggests several possible reasons for these deviations, including adsorbed immobile water near clay surfaces, non-Newtonian fluid behavior in nanopores, and induced streaming potential or electroviscous effects. At nanoscales, the impact of the molecular interaction forces between fluids and solids becomes increasingly significant, influencing fluid phase behavior and transport properties. This study incorporates intermolecular, surface tension and surface forces including electrostatic interactions into a pore-scale model based on classical density functional theory. We present preliminary applications of the model to understand macroscopic flow properties, such as water permeability, in a computer-generated nanoporous medium containing multiple clay particles.

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Poster / 246

Anomalous Transport in Dissolving Porous Media: Transitions Between Fickian and Non-Fickian Regimes

Authors: Jingxuan Deng^{None}; Peter Kang¹; Piotr Szymczak²; Rishabh P. Sharma³

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Mineral dissolution is a key geologic process that can control many natural processes and human activities. Depending on the interplay between advection, diffusion, and reaction rates, mineral dissolution can produce various dissolution patterns, such as wormholing and uniform dissolution. The resulting changes in pore structure directly influence the flow field, which in turn control solute transport behavior. In this study, we conducted numerical modeling of mineral dissolution and solute transport in pore networks to investigate how initial network heterogeneity and dissolution regimes affect transport dynamics.

Dissolution of porous media is simulated using a 2D pore network model in which a porous media is represented as a series of interconnected cylindrical tubes with diameters getting enlarged in proportion to local reactant consumption. The heterogeneity is introduced in a network by assigning initial diameters to the tubes from log-normal distribution. The networks were subjected to varying dissolution regimes, from homogeneous to wormholing, resulting in changes in network heterogeneity. To investigate and analyze the impact of dissolution on the transport behavior, passive tracer transport simulations were performed using particle tracking.

Our findings show that dissolution significantly influences transport behavior by modifying the network's heterogeneity. In the wormholing regime, formation of highly conducting flow channels and stagnation zones increases network heterogeneity, resulting in the transition from Fickian to non-Fickian transport in networks with initially homogeneous structures. Conversely, in the uniform regime, reactant extensively homogenize the pore network and the flow field, leading to the transition from non-Fickian to Fickian transport, even in networks with high initial heterogeneity. We investigate the detailed mechanisms governing the transitions and show that the transitions could be predicted based on the initial network heterogeneity and Damköhler number.

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MS10 / 247

Deposition of droplets on inclined porous surfaces

Authors: Dominique Derome¹; Jan Carmeliet²; Maude Dias^{None}

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Water infiltration in buildings is an increasing issue that has intensified with climate change : weather conditions (floodings, storms) are progressively becoming more intense and may cause a faster deterioration of buildings. In order to analyze the consequences of wind driven rain on built materials, the impact of rainfall on an inclined porous surface is observed at droplet scale. The droplet spreading dynamics are recorded on high speed cameras from two points of view.

The shadowgraphy technique is used to observe the droplet fall and spreading through the high speed camera with great contrast and lightning. A direct light is placed facing the camera in order to observe only the shadow of the drop, which allows to accurately measure its diameter while it is falling and spreading. The cameras are set at a precise distance to capture the drop impact and maintain sufficient resolution. An optical zoom lens is set up to seize the complete droplet spreading in any regime: deposition, bouncing or splashing. The camera setup, spatial and time resolution, allows to record the spreading and beginning of absorption process of the impinging drop.

Some characteristics of both the liquid and the porous surface are determined, in order to draw a phase diagram that weighs the importance of the different parameters. Some of them are the droplet diameter, the viscosity and surface tension of the liquid, the porosity of the surface. The high speed cameras allow to record the spreading diameter of the droplet and its surface to obtain the dynamic surface energy. The velocity of the droplet and the angle of impact are the two varying parameters. With an energy equilibrium model, the dynamic parameters are linked to the set characteristics, in order to predict the spreading ratio. A few hypotheses take into account the spreading shape of the droplet, to simplify the surface energy, that is compared to the experimental data. The experimental data agrees with the correlation obtained theoretically. Understanding porous surface wetting by a single droplet is essential to upscale the analysis. Analyzing the droplet behavior throughout the spreading and absorption process is necessary to quantify the moisture content of the substrate and what surface is affected. This has to be considered in order to estimate the area potentially contaminated by the droplet and to better understand the drying mechanism of building materials. The effects of a droplet spreading can help to predict the wetting, drying and runoff of rain water in the built environment at urban scale.

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MS14 / 248

Solving inverse problems with machine learning for real-time monitoring of subsurface plumes

Authors: Alice Nuz¹; Gege Wen²; Sally Benson³

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There is an immediate need for carbon sequestration coupled with a need for low-cost, continuous monitoring, and real-time awareness of the saturation plume to prevent leakage. We seek to maximize plume prediction accuracy with economical and reliable monitoring strategies. Multilevel pressure monitoring is a monitoring scheme shown to be effective in determining the height and footprint of a plume. An approach directly inverting saturation maps is considered. A machine learning model is trained with an augmented U-Net architecture to history match a single deterministic full saturation map using input well data. A machine learning forward model with U-FNO

architecture is used in conjunction with the direct inversion approach to generate a stochastic ensemble of full saturation maps. The direct inversion approach is shown to be effective, achieving close statistical agreement with the ground truth. For the direct inversion model, a base model is trained using permeability, porosity, and pressure buildup well data. The plume error over the 500 sample test set was 2.019%. The benefits of this approach over traditional history matching are computational efficiency, the ability to generalize out of sample, and not being dependent on priors. We produce ensembles of saturation maps that can learn the height and footprint of the plume and reasonably reconcile observed pressure data with predicted pressure data over time while incorporating uncertainty quantification from both measurement error and model error into predictions.

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MS06-A / 250

Quantification and modeling of pore-scale foam behavior

Authors: Masa Prodanovic¹; Xuesong Ma^{None}

¹ *The University of Texas at Austin*

Corresponding Authors: masha@utexas.edu, cedar996@utexas.edu

Foam diversion effect is potentially useful for mobility control in both dioxide storage and enhanced oil recovery processes in subsurface. The transport behavior of foam at pore scale in the porous media has thus far been mostly studied using micromodels (i.e. experimentally) and pore-scale numerical models have lagged behind.

We have recently introduced a pore-scale model for foam based on lattice Boltzmann method (Ma, Chang, and Prodanović 2024). The model is capable of capturing bubble nucleation and growth during the generation stage, followed by bubble deformation during flow owing to shear, as well as coalescence and trapping ascribed to solid wall roughness during. This model is able to import any imaged geometry (e.g. from micro-tomography) as the solid boundary. While we have mostly used the model in 2D, 3D model has been implemented alas it is computationally expensive.

We here focus on validating this model by direct comparison to two micromodel experiments, and find that the numerical results obtained in this work are accurate and in good agreement with the literature using the microfluidic device. We further investigate pressure buildup, foam texture, the influence of foam quality and capillary number on foam apparent viscosity during foam flow. Results also indicate that the calculated foam apparent viscosity is approximately five times higher than the water viscosity when traversing a smooth fracture. The simulations capture the effect of changing bubble size, capillary number, and pore geometry. We finally simulate foam behavior while approaching a system of two different, parallel fractures and show that higher bubble density helps boost foam diversion to fractures associated with larger apertures.

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Ma, Xuesong, Bernard Chang, and Maša Prodanović. 2024. "Direct Pore-Scale Modeling of Foam Flow through Rough Fractures." *Energy & Fuels* 38 (15): 14449–60. <https://doi.org/10.1021/acs.energyfuels.4c01664>.

Poster / 251

Quantifying the yield envelope of geomaterials at elevated temperatures

Author: Kaina Rodrigues Vieira¹

Co-authors: Geng Niu¹; Laura Dalton¹; Qinyi Tian ; SONIYA Tiwari

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Plasticity is the study of plastic deformation of materials, which can be quantified using governing and constitutive laws including the conservation of mass, conservation of moment, conservation of energy, and the second law of thermodynamics. A major challenge civil engineers face today is ensuring infrastructure built in coastal environments remains durable, adaptable, and resilient to a changing climate. Chlorides and sulfates are omnipresent in coastal environments and permeate into Portland cement-based infrastructure which leads to chemical restructuring and can alter the mechanical behavior for which the structure was designed to withstand. The objective of the current study is to analyze the mechanical behavior of bentonite clay and Portland cement concrete materials at incremental loading regimes and temperatures to assess the impact of thermal fluctuations on the mechanical behavior of each material. Before running the experiments, a high-resolution X-ray micro-computed tomography (CT) scan will be completed to obtain a 3D model of each sample. For the mechanical test, the Environmental Triaxial Automated System (ETAS) will be used to perform incremental loading to obtain the Young's Modulus and yield envelope of each material at three temperatures: 20, 50, and 80 °C. The samples will remain inside the rubber sleeve after testing and rescanned using the same X-ray micro-CT parameters to obtain a 3D volume of the failed sample. The results from this initial study will help guide subsequent experiments that will integrate samples exposed to salt solutions and address solutions to the modeling and design of structures built in aggressive environments.

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MS06-A / 252

Nonequilibrium multiphase flow and thermodynamic phase change in nanoporous shale rocks: Pore-level physics, network modeling, upscaling

Author: Sidian Chen¹**Co-authors:** Jiamin Jiang²; Chaozhong Qin³; Bo Guo⁴¹ *Stanford University*² *University of Science and Technology of China*³ *Chongqing University*⁴ *University of Arizona***Corresponding Authors:** boguo@arizona.edu, sidianc@stanford.edu, chaozhong.qin@cqu.edu.cn, jiaminjiang@ustc.edu.cn

Unconventional shale oil and gas plays an important role in the global energy transition. However, predicting oil and gas production from shale formations remains a critical challenge, largely due to the abnormal thermodynamic phase change behavior and nonequilibrium multiphase fluid flow within the extensive nanometer-scale pore spaces in shale rocks. While the abnormal behaviors have been extensively studied in a single nanopore or a few nanopores, its manifestation in complex nanopore networks remains poorly understood and rigorously derived macroscopic phase behavior formulations are not yet available. To address these challenges, we have developed a group of (static and dynamic) pore-network models that can represent the resolved nanopore spaces in shale rocks and account for molecular-level phase change and multiphase fluid flow processes therein. Our simulations highlight the critical role of pore size distribution in upscaling single-nanopore phase behavior to core-scale, and reveal the importance of the coupling effects between thermodynamic phase change and multiphase fluid flow. These advancements provide a foundation for integrating pore-scale physics into reservoir-scale models, offering a powerful tool to optimize shale energy production for advancing energy transition.

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Poster / 254

Semi-analytical solutions for nonequilibrium PFAS transport in heterogeneous vadose zones

Author: Sidian Chen¹**Co-author:** Bo Guo²¹ *Stanford University*² *University of Arizona*

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We present screening-type models for quantifying the fate and transport of perfluoroalkyl acids and their precursors (PFAS) in a heterogeneous vadose zone. The models represent the heterogeneous vadose zone by one-dimensional dual-porosity, dual-permeability, or tripe-porosity domains. They account for transport mechanisms specific to PFAS and their precursors—including multi-site rate-limited solid-water and air-water interfacial adsorption and biochemical transformation. Assuming steady-state infiltration, linear adsorption, and first-order-rate transformation, we derive semi-analytical solutions for these models under arbitrary initial and boundary conditions. The newly derived solutions have been validated by experimentally measured breakthrough curves of PFAS and other solutes for various soils and wetting conditions. Additionally, we demonstrate the models' capability for analyzing long-term PFAS leaching and mass discharge in a heterogeneous vadose zone beneath a PFAS-contaminated site. Among other findings, the simulations show that the strong retention of PFAS (especially longer-chain PFAS) reduces the mass-transfer limitations and non-equilibrium transport behaviors between the different pore domains. Overall, the semi-analytical models provide practical tools for assessing the long-term fate and transport of PFAS in the vadose zone and for soil screening applications.

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MS08 / 255

Fracture regulates statistical steady-state Rayleigh-Darcy convection pattern in porous media

Author: Jingwei Zhu^{None}

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When concentration or temperature contrast results in higher fluid density at the top of a porous stratum than that at the bottom of a porous stratum, buoyancy may drive Rayleigh-Darcy (R-D) convection that fundamentally shapes the transport and reactive dynamics. R-D convection commonly emerges in CO₂ sequestration and in stratums with high geothermal gradient. Regardless of numerous studies on flow pattern and transport kinetic model in homogeneous media, the effect of heterogeneity (especially the emergence of fractures) on R-D convection is largely under debate. Here, we study how a single vertical fracture shapes the flow field during R-D convection at steady-state. We adopt Lattice Boltzmann modeling method with two coupled Lattice Bhatnagar-Gross-Krook (LBGK) models. We vary Rayleigh number (characteristic ratio of gravitational-driven flow flux over molecular diffusion flux) from 500 to 6000, fracture volume fraction from 6.25% to 23.86%, and fracture-matrix permeability ratio from 1.01 to 451. Flow patterns are recorded with the system falls to statistical steady state. Surprisingly, most numerical simulations show consistent pattern: high-density fluid mainly flows

down through the fracture, whereas the low-density fluids go upward through the matrix. We propose a simple theory that the flow pattern is determined by minimization of total gravitational potential energy leads to this flow pattern. We establish a toy theoretical criterion, that well predicts the flow pattern calculated from numerical simulation. This criterion can be extended to other heterogeneous media than fractured media.

This successful and theoretical approach on simple system demonstrates how geometrical heterogeneity reduces fluid flow uncertainty. In the future, we will investigate heat & mass transport during R-D convection in more complicated systems.

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MS11 / 256

Microbial transport toward residual chemical contamination trapped in low permeable regions of a microfluidic device with layered structural heterogeneity is optimal at moderate Peclet numbers

Author: Beibei Gao¹

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Groundwater pollutants that become trapped in low-permeable clay lenses are difficult to remediate using conventional pump-and-treat methods. Water flows preferentially through more permeable sandy layers leaving behind residual contamination in clay lenses that then slowly leaches out over time creating a long-term contamination problem. An alternative approach to pumping contaminants above ground for treatment is to deliver microorganisms that biodegrade the chemical pollutants in place. Chemotactic bacteria can swim from the highly permeable layers to access residual contamination that is trapped at the boundaries of low-permeable layers. These bacteria detect the presence of chemical pollutants and migrate toward increasing concentrations to accumulate at the source.

To analyze the complex interactions between fluid flow, bacterial transport, and contaminant transport in porous media for this scenario, we used a microfluidic device designed with a highly permeable region sandwiched between two low-permeable layers representing clay lenses within a sandy aquifer. A chemical pollutant (naphthalene) dissolved in a non-aqueous phase liquid (NAPL) was flushed from the device leaving behind residual droplets, especially at the boundaries between the high- and low-permeable layers. A suspension of bacteria chemotactic toward naphthalene (*Pseudomonas putida* G7) was then flowed through the device. Pore-scale imaging was used to quantify accumulation of chemotactic bacteria near the residual contamination over time at several positions along the length of the microfluidic device. Experimental observations over a range of fluid velocities and pore configurations were compared to computer simulations of Darcy-scale transport equations solved for the microfluidic device geometry.

Our analysis revealed an optimal fluid flow velocity for bacterial accumulation that balanced fluid penetration into dead-end pores blocked by residual NAPL and bacterial transport by chemotaxis

within the quiescent fluid of those dead-end pores. We initially expected as the fluid velocity increased bacterial accumulation would decrease monotonically because the independent swimming motion of chemotaxis was overcome by convective flow. However, what we found was a more complex role of fluid velocity that increased accumulation and complemented chemotaxis up to a maximum value before decreasing as originally anticipated. We found that bacterial accumulation in the vicinity of residual naphthalene-containing NAPLs was greatest for values of a chemotactic Peclet number around 10.

To relate our laboratory-scale observations to larger-scale field studies we used dimensional analysis. Simulated outcomes from the microfluidic device over a range of velocities, observation times, and positions along the flow path were fit to a logistic equation using dimensionless parameters. Bacterial transport dynamics were effectively described by two timescales, one associated with fluid flow and one with chemotaxis, highlighting that directed migration in porous media can be determined by two key processes: convection that carries bacteria to the vicinity of contaminant sources and chemotaxis that is driven by pore-scale chemical gradients.

Outcomes from our study suggest that flow rates for pump-and-treat scenarios may be adjusted to maximize bioavailability of residual contaminants for chemotactic bacteria.

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Pore-scale modeling and simulations of microbially induced carbonate precipitation in 3D geologic media through the micro-continuum approach

Authors: Xiaofan Yang¹; Xueying Li^{None}; Xiaowei Chen²

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Microbially induced carbonate precipitation (MICP) is a biologically driven mineralization in geologic media, during which the metabolic activity of microorganisms generates urea and further produces CO_3^{2-} , forming calcium carbonate precipitation with free Ca^{2+} . It serves as an emerging eco-friendly technology in areas such as bioremediation, petroleum extraction, and particularly carbon capture, utilization, and storage (CCUS). The MICP processes are highly coupled and complex, and its efficiency is significantly affected by the topology of the geologic media and the environmental conditions in the pore space. A major challenge for modeling MICP in 3D geologic media is the integration of coupled biogeochemical processes into a cohesive set of equations, while also capturing the evolution of porosity and permeability. Recent experimental studies reveal that the 3D topology is critical to control reaction dynamics by redirecting the velocity field, while flow fluctuations affect biomass accumulation, indicating the potential impact on MICP behavior. However, most numerical models simulate MICP in 2D porous geometries and cannot determine the optimal environmental conditions for MICP efficiency.

This study develops a new 3D MICP solver, *micpFOAM*, by using the micro-continuum approach implemented within the OpenFOAM environment. After point-by-point validation against existing experimental and numerical data, the model is applied to simulate 3D MICP processes in various configurations, including a single pore, a beads pack, and a realistic media of quartz sand extracted from XCT scanning. Results show that the effects of secondary flow lead to biomass fluctuations caused by flow instabilities. Structural heterogeneity enhances the secondary flow, further alleviating MICP efficiency. We also evaluate several environmental factors that could improve MICP efficiency. Results show that greater biomass and more homogeneously distributed initial microbial attachment result in higher MICP efficiency. Higher temperatures and pH levels increase MICP efficiency by increasing ureolysis and precipitation rates. However, both rates being high can result in anomalous transport behaviors that reduce MICP efficiency, while a combination of fast precipitation ($K_p = 10^{-2}$) and low ureolysis ($K_u = 10^{-5}$) promote MICP. This model highlights the significant role of secondary flow and environmental factors on MICP behavior, offering an applicable framework for optimizing the MICP efficiency in fields like bioremediation and CCUS.

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MS01 / 258

Effects of Aquifer Salinity on Underground Hydrogen Storage

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Underground hydrogen storage (UHS) is a promising technology for enabling large-scale clean energy resilience. Deep saline aquifers, known for their abundance and ample storage capacity, are promising sites for UHS. Despite considerable research on the technical feasibility of UHS in saline aquifers, a significant knowledge gap persists regarding the impact of aquifer salinity on UHS performance. To bridge this gap, we conducted high-fidelity reservoir simulations to quantitatively evaluate the effects of salinity on three critical UHS performance metrics: the maximum reservoir pressure buildup, the liquid-gas ratio of the produced fluids, and the hydrogen withdrawal efficiency. Our results indicate that aquifer salinity significantly impacts the UHS performance. Hydrogen injection into saline aquifers can desiccate the near-well formation, causing salt precipitation that reduces the formation porosity and permeability. Under the geological and operational conditions of our simulations, the precipitated halite is mostly dissolvable in aquifers with a salinity not exceeding 10%, causing only minor permeability reduction. Within this range, an increasing salinity can benefit UHS performance by decreasing the produced liquid-gas ratio and improving the hydrogen withdrawal efficiency, without significantly raising the maximum reservoir pressure buildup. However, when the aquifer salinity rises to 15% or higher, UHS operations suffer from massive halite accumulation during successive storage cycles. Such accumulation elevates halite saturation, severely clogging

the near-well zone, drastically increasing the maximum reservoir pressure buildup, and reducing hydrogen withdrawal efficiency. To our knowledge, this is the first study to evaluate the effects of aquifer salinity on UHS performance at the field scale. Our proposed simulation workflow can be applied to any saline aquifer targeted for UHS, yielding useful insights for site selection, design, and operational management of future UHS projects.

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MS25 / 260

Oscillating Flow Leads to Sustained and Enhanced Mixing-Induced Mineral Precipitation in Porous Media

Authors: Weipeng Yang¹; Tomasz Szawello²; Piotr Szymczak²; Peter Kang¹

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Mixing-induced mineral precipitation significantly influences various natural and engineered processes such as carbon mineralization, aquifer recharge, and enhanced geothermal systems. Traditionally, this process has been viewed as self-limiting due to the formation of a thin precipitate layer along the mixing interface, which inhibits further fluid mixing and subsequent precipitation [1]. However, our recent work shows that fluid inertia can significantly enhance mixing-induced precipitation [2]. In this study, we introduce a novel mechanism whereby oscillatory flow sustains and dramatically amplifies mixing-induced mineral precipitation in porous media, even under creeping flow conditions.

We performed microfluidic experiments and pore-network modeling to explore the impact of oscillating flow on mixing-induced mineral precipitation in porous media. Barium chloride and sodium sulfate solutions were co-injected into porous microfluidic chips at an oscillating injection rate, maintaining a constant total flow rate and a 10% flow rate difference between the two solutions. The flow rate between the two inlets alternates every 30 minutes, ensuring periodic flow rate oscillations. Precipitation dynamics were captured in real-time using an inverted fluorescence microscope with brightfield imaging, while fluid mixing was characterized through fluorescence imaging. Additionally, X-ray micro-CT scans provided detailed 3D morphology and spatial distribution of the precipitated minerals. Our results demonstrate that oscillating flow conditions prevents the formation of a mixing barrier and actively enhances transverse precipitation across the porous media. As the flow oscillates, precipitation continuously expands transversely, resulting in a broad precipitation zone with porous precipitates. This is in contrast to the thin, dense precipitation layer formed under steady flow conditions. X-ray micro-CT images confirm that the precipitates exhibit microporosity, resulting in dual porosity and a heterogeneous permeability field. These experimental findings align closely with the pore-network modeling results, validating the observed phenomena.

This study highlights the crucial role of flow conditions in controlling spatiotemporal dynamics and patterns of mixing-induced precipitation in porous media. These findings have important implications for various natural and engineered processes where understanding and control of mineral precipitation is critical.

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USA

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MS01 / 261

Techno-economic assessment of a novel hybrid plant for solar thermal hydrogen storage in subsurface systems

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Grid stability and reliability problems related to renewable energy sources have hindered the transition to an eco-friendly future. Solar Power Tower (SPT) plants mitigate local, short-term energy supply fluctuations by achieving high thermodynamic cycle efficiency and employing thermal energy storage tanks to reuse excess heat later. Nevertheless, tackling long-term intermittency issues at regional and even global levels, coupled with the anticipated rise in energy demand, necessitates large-scale solutions. The integration of underground hydrogen storage (UHS) systems with SPT plants presents a promising strategy for significant energy storage, supporting various industries. High direct normal irradiation (DNI) values in California and Texas, combined with the abundance of suitable UHS sites, make this hybrid facility highly applicable. However, the potential financial returns of this hybrid approach, with federal tax incentives, have yet to be determined. Therefore, the research aims to conduct a techno-economic comparative analysis between salt caverns and depleted reservoirs to evaluate the viability of the novel SPT-UHS model within the USA.

The case study utilises the Aliso Canyon natural gas storage field in Southern California as a depleted reservoir for the UHS. After calculating its total working gas capacities, a system comprising multiple salt caverns is developed in the Permian Basin, West Texas, to achieve an equivalent capacity. Due to geological constraints and the limited availability of regions with high DNI, the SPT plant in each hybrid model is located inland at a moderate distance from the UHS site. The pure water required for a thermochemical Cu-Cl electrolysis process is obtained through the desalination of local aquifer water sources. To improve electrolyser efficiency, a photovoltaic (PV) station provides the necessary electricity for hydrogen (H₂) production and compression for subsurface injection at a specific SPT:PV ratio. Additionally, oxygen (O₂), a byproduct of electrolysis, is assumed to be sold to hospitals to increase profits.

The primary contribution of this research is a full techno-economic analysis of the SPT-UHS hybrid system, yielding extremely advantageous financial outcomes. The SPT configuration, with a gross capacity of 270 MW, supplies H₂ to 69 salt caverns, attaining the same working capacity in kg of the single depleted reservoir. The findings indicate that the highest net present value (NPV) and the

shortest payback period (PBP) for the salt cavern system are approximately USD 7.4B and 6 years, respectively, while for the depleted reservoir, these values are around USD 8.8B and 4 years. The existing literature predominantly focuses on wind-UHS hybrid plants, which exhibit NPVs below USD 17MM. Compared to the system analysed in our study, their PBPs are extended by a factor of 2.1 for salt cavern storage and 1.6 for depleted reservoir storage. This highlights the benefits of the large-scale SPT-UHS facility with both O₂ sales and storage schemes. Although selling H₂ generates higher net cash flow, the sale of O₂ has a greater impact on NPV by enhancing the project's financial stability. Furthermore, applying tax incentives and O₂ sales boosts the SPT-UHS system's economics, reducing PBPs by 6% and 49%, respectively, resulting in a combined 54% improvement.

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Transport, packing stability and long-term conductivity of proppant in the multiscale fractures of shale

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Hydraulic fracturing is one of the key stimulation technologies of Gulong shale, Qingshakou Formation, China. Proppant has always been a vital part in the hydraulic fracturing operation, as it supports the fracture against the closure stress. A successful delivery of the proppant to the aiming fracture, as well as a long-term propping effect to a great extent determines the reservoir permeability and well productivity. This requires a well-projected selection and injection scheme of proppant, from which an optimised proppant distribution and thus fracture conductivity could be achieved.

Hence, the main aim of the current research is to perform a systematic investigation of proppant, from its injection to the fracture network to the long-term fracture conductivity. To achieve this, we conduct both experimental and numerical studies to seek for an optimised proppant injection scheme as well as a critical packing ratio with which the fracture permeability reaches the maximum. The numerical study is accomplished by the implementation of the numerical framework consisting of the lattice Boltzmann method (LBM) and the modified partially saturated method (MPSM). As an extension to our previous study where Queensland coals were investigated, we apply the mechanical parameters of the Gulong shale to our model. The results indicate an optimised proppant packing ratio of 0.2 - 0.4. The fracture conductivity is experimentally evaluated using the shale cores and sand proppant at the reservoir pressure. The GCTS tri-axial testing system is utilised to conduct the experiments. By adjusting the proppant packing ratio, we find an optimised proppant concentration, under which the fracture permeability reaches the maximum. Besides, the final distribution of proppant using different injection schemes are experimentally studied. The long-term fracture conductivity of these distribution patterns is further evaluated using a core testing holder under overburden pressure, from which a long-term conductivity curve is obtained.

The outcome of the current research contributes to a better design of the proppant and the resultant fracture permeability especially for shale. It also provides a theoretical basis for an optimised proppant selection and injection scheme for future hydraulic fracturing operations, which benefits the exploitation of the continental shale oil worldwide.

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MS01 / 264

Microfluidic Study of the Pore-Filling and Propagation Behaviors of CH₄ and CO₂ Hydrates in Porous Media

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Gas hydrates are crystalline solids in which guest molecules are trapped within cages formed by water molecules under high-pressure and low-temperature conditions. The phase transition of hydrates, as well as the transport behaviors of the associated gas and liquid phases in porous media, is crucial for CH₄ production and CO₂ storage using hydrates. In this work, we investigate the phase transition behaviors of CH₄ and CO₂ hydrates within porous media under realistic oceanic conditions. To study pore-filling behaviors and spatial stochasticity during hydrate formation in porous media, we developed a low-temperature, high-pressure (LTHP) microfluidic system. This system enables simultaneous visualization of hydrate phase transitions at both the pore and chip scales. It allows for detailed pore-scale morphological studies and observation of collective hydrate formation and propagation behaviors across an area of 45 × 30 mm, etched with over 18,000 pores. To the best of our knowledge, this is the first study of its kind to offer dual-scale imaging over such a large field of view in porous media. Our study reveals density-dependent pore-filling behaviors during gas hydrate formation, addressing knowledge gaps left by earlier microfluidic studies. Hydrates formed from lighter phases, such as gaseous CH₄ and CO₂, partially fill pores by coating pore walls upon reaching equilibrium. In contrast, hydrates formed from denser phases, like liquid CO₂, rapidly cement the pores due to volume expansion, significantly reducing the permeability of the host material. This pore-filling phenomenon was visualized using fluorescence imaging and analyzed through the volume variation index, with kinetics examined under various conditions. We uncovered intrinsic spatial stochasticity in hydrate formation within porous media, demonstrating a random distribution of newly formed hydrates. This randomness can be mitigated through an injection process that simulates CO₂ storage, promoting directional hydrate propagation along pressure gradients. Lastly, we propose an alternating CO₂-water injection method to enhance CO₂ storage capacity and injectivity in shallow seabed environments.

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MS09 / 268

Particulate transport in porous media at pore-scale**Author:** Laurez Maya¹**Co-authors:** Laurent ANDRE²; Philippe Leroy²; Cyprien Soullaine³¹ BRGM - ISTO² BRGM³ CNRS**Corresponding Authors:** l.andre@brgm.fr, laurez.maya@cnrs-orleans.fr, cyprien.soullaine@cnrs.fr, p.leroy@brgm.fr

Particulate transport and retention in porous media are crucial processes influencing permeability reduction and clogging, particularly in natural and industrial systems. In this work, we present a novel hybrid Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) approach that combines unresolved and resolved coupling strategies [1]. This innovative method allows the simulation of particulate flows across complex pore geometries, accommodating particles of varying sizes relative to the computational grid. Our model efficiently identifies grid cells interacting with particles and accurately computes the fluid-solid momentum exchange term, ensuring robust and efficient simulations. The model further incorporates colloidal forces using the DLVO (Derjaguin-Landau-Verwey-Overbeek) theory and adhesive contact forces based on the Johnson-Kendall-Roberts (JKR) model to account for electrochemical interactions (e.g., Van der Waals attraction, electrostatic double-layer repulsion) and particle adhesion dynamics [2]. Coupled with hydromechanical forces (e.g., drag, buoyancy, collision), the model enables realistic pore-scale simulations of particle transport, sieving, bridging and aggregation phenomena. The robustness and accuracy of our CFD-DEM framework are demonstrated against reference analytical and experimental cases. We showcase its capabilities by investigating pore-clogging and permeability reduction under varying conditions, such as fluid salinity, particle size distribution, concentration, flow rates, and pore geometry. Unlike conventional approaches, this hybrid model is not constrained by particle size relative to the grid, offering enhanced flexibility and reliability for simulating particulate transport in porous media. This work paves the way for improved understanding of pore-scale mechanisms and their impact on macroscopic flow properties.

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Poster / 269

Evaluation of Entrained Air Void Structure in Fly Ash Concrete Using Foam Index Test and 4D X-ray Micro-CT

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Coal combustion ash (CCA), specifically fly ash, is a supplementary cementitious material (SCM) used in the construction industry to lower the carbon footprint and the cost-efficiency of concrete production. However, the inclusion of CCA introduces challenges to achieving adequate air void (i.e., large pore) structure because of the adsorption of the air entraining admixtures (AEAs) by the excess unburned carbon in CCA and the high fineness (i.e., high specific surface area) of ash particles. In this study, we investigate the relationship between the results of the Foam Index (FI) test and the resulting air void structure in hardened fly ash concrete. The FI test (ASTM C1827-20) is the standard method used to determine the optimal AEA dosage required to attain the target air void content in slurry form. Cylindrical concrete samples were then generated using the results from the FI test and X-ray micro-computed tomography (CT) scanned (Figure 2a) to obtain high-resolution 3D visualizations as a function of the curing time of the internal air void structure in both the transition to and final hardened concrete. Advanced image processing techniques were then employed to calculate the 3D spacing factor among the air voids, a critical parameter for assessing freeze-thaw durability. The analysis offers detailed insights into pore distribution, and the influence of fly ash properties on air void content and concrete performance. By integrating experimental methods like foam index testing with computational analysis using X-ray CT imaging, this research provides a comprehensive approach to optimizing air entrainment in fly ash concrete. The findings contribute to the development of more durable construction materials and offer practical guidance for incorporating supplementary cementitious materials into concrete design.

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MS09 / 272

Upscale rarefied volatile diffusion in porous media: a probability-based pore network modeling approach

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In certain regions of airless bodies, such as the Moon and cometary nuclei, volatile components like water, carbon dioxide, and methanol can persist and migrate within the regolith due to extremely low temperatures[1-5]. Studying the diffusion behavior of volatiles in porous media is crucial for the exploration and exploitation of these extraterrestrial resources.

Under such extremely high vacuum conditions[6], gas molecules undergo Knudsen diffusion, where the average free path is more than 10 orders of magnitude larger than the size of regolith particles[7] (Knudsen number $Kn > 1010$). At this almost infinitely large Knudsen number, gas molecules rarely collide with each other, and the diffusion trajectories resemble chords (free paths) between solid surfaces, determined solely by porous structure. Additionally, the number of molecules within a single pore is too small to satisfy statistical continuity. Previous studies on Knudsen diffusion have been limited to either simple tube-like structures[8-11] or Monte Carlo simulation[12, 13] that only provide chord length distributions and effective diffusion coefficients. A direct model linking pore structure to dynamic diffusion behavior is still lacking.

We first conduct numerical experiments by employing test particle Monte Carlo (TPMC) simulations, to obtain molecular trajectories and the diffusion coefficients in complex porous media. We find that pore-bodies and pore-throat behaves very differently. Pore-bodies exhibit isotropy (the exit direction of molecules in pores is uniformly distributed) and satisfy the Markov property (the exit probability of molecules in pores is independent of their residence time), while pore-throats are anisotropic and do not satisfy Markov property.

Based on this duality of local diffusive property and the rarefied feature, we develop a probability-based pore network modeling (pb-PNM) approach to upscale Knudsen diffusion from pore-scale to representative elementary volume (REV) scale. The model uses the probability of a molecule residing in a specific structure (i.e., pore or throat) at a given time to represent the spatial distribution and transfer probability of a molecule between different structures to represent the change in the spatial distribution within a specific time period. The relative error between the predicted diffusion coefficient and the numerical experimental results is less than 20% in most cases.

This pb-PNM method leverages the characteristics of gas molecular movement in pores and throats, obtained from TPMC simulations, to scale up to larger core scales. As a result, this method can be used to analyze the effects of adsorption and heterogeneity on the diffusion of rarefied volatiles, and to simulate the unsteady diffusion process with significantly fewer computational resources compared to TPMC simulations.

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MS15 / 273

PoroNet: An Interpretable Pore Graph Neural Network for Prediction of Gas Adsorption in Nanoporous Materials

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Machine learning (ML) models have been widely used as efficient surrogates for costly molecular simulations to predict gas adsorption in nanoporous materials for gas storage and separation applications. The “black box” nature of ML, however, often limits its ability to guide the discovery and design of novel nanoporous materials. In this work, we introduce PoroNet, a new graph neural network architecture built on a graph representation of the pore network (i.e., pore graph). In a pore graph, nodes represent individual pores and edges represent pore connections. PoroNet shows highly accurate predictions of gas adsorption capacity on benchmark datasets, which include the simulated adsorption data of spherical molecules (Kr and Xe) and linear alkane molecules (ethane and propane) in metal-organic frameworks (MOFs) under various pressures and temperatures. More importantly, pore-level contribution to the adsorption can be learned using PoroNet through both direct supervised learning and as an emergent property while optimizing the total adsorption capacity. In the direct supervised learning experiments, we show that PoroNet is data-efficient, achieving comparable performance to the standard approach with only a fraction of the training data. These pore-level contributions help explain the ML predictions of the total adsorption behavior and can provide significant insights into pore engineering. We demonstrate that PoroNet is a powerful tool for high-throughput MOF screening and derivation of valuable design rules for hydrogen storage applications.

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MS03 / 274

Fracture initiation of polymer flooding using CFD-DEM model in porous media

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In this work, we have studied numerically the fracture initiation conditions induced by non-Newtonian polymer solution in the granular media. Computational Fluid Dynamics (CFD) coupled with the Discrete Element Method (DEM) technique is used to model fluid flow through porous media. The power law used to describe the polymer solution flow. The associated parameters are considered in the drag force computation for CFD-DEM framework. The numerical model is validated by the laboratory experimental data [1]. The results of the different polymer solutions are presented in the proposed criteria of fracture initiation. The impact of fluid rheology, injection rate, stress conditions, and granular material parameters on the fracture model is presented.

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Kazakhstan

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Poster / 276

FE-SEM observation of gypsum precipitation in wellbore cement exposed to CO₂ under geologic carbon storage conditions

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Wellbore cement serves as a critical barrier to prevent the migration of CO₂ through the wellbore and to the surface in CO₂ geological storage sites. However, the cement may exhibit chemical instability under CO₂-rich conditions. This research examines the changes in the pore structure of reaction zones within wellbore cement samples that have been subjected to a CO₂-rich solution equilibrated with 17 MPa supercritical CO₂ for a period of 14 days. Utilizing sophisticated characterization techniques such as Field Emission Scanning Electron Microscopy (FE-SEM), Quantitative Evaluation of Minerals by Scanning Electron Microscopy (QEMSCAN), and Micro-computed Tomography (micro-CT), a novel mechanism of CO₂-cement interaction has been discovered and elucidated. This mechanism involves the filling of nanopores within the cement matrix by gypsum. Gypsum formation is attributed to the release of SO₄²⁻ ions from ettringite (AFt) and monosulfate (AFm) phases, which

is induced by a reduction in pH. Based on these experimental findings, an improved CO₂-cement reaction model has been developed, incorporating four distinct reaction zones. This model offers a comprehensive framework for understanding the spatial and temporal distribution of minerals in cement resulting from high-pressure and high-concentration CO₂-cement interactions. This study indicates that the primary damage caused by high-pressure CO₂ corrosion occurs in the outermost region of the cement. The inner region of the cement retains its structural integrity due to the filling of nanopores by gypsum.

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Correlation between mass transfer and laplace pressure effects in immiscible spatio-temporal invasion dynamics in asymmetric pore throat distribution

Author: Debanik Bhattacharjee^{None}

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Immiscible phase flow in porous media occurs in various applications, like unsaturated soil, non-aqueous phase (NAPL) remediation, and oil recovery. In these processes, an immiscible invading fluid displaces a defending fluid within the confines of a heterogeneous porous structure, yet the invasion pattern continuously evolves over time due to the chemical action of surfactants that alter the interfacial tension and surface wettability. We develop a time-dependent pore network model (PNM) to simulate the effects of surfactant-induced IFT reduction on two-phase flow under constant driving pressure. The initial invasion follows invasion percolation theory, with pressure drops across the network calculated using a random resistor network and mass conservation equations. Node-specific flux and velocity are derived using the Hagen-Poiseuille law. Surfactant adsorption is modeled using Langmuir kinetics, capturing its impact on fluid-fluid and solid-fluid interfaces within the invaded path. Over time, the reduced IFT and alterations in contact angles trigger secondary invasions, reshaping the invasion patterns. The model explores the correlation between mass transfer effects and dynamic Laplace pressure as the skewness (median/mean ratio) of the pore size distribution increases. This dynamic behavior aligns with Kosugi's framework [1,2], emphasizing the significance of IFT change. Results indicate that with symmetric pore size distribution, invasion patterns evolve more strongly due to mass transfer effects compared to Laplace pressure.

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MS11 / 278

Multiscale Analysis of Coupled Free-Flow and Porous Media Systems: Structured and Random Configurations

Author: Mario Del Mastro^{None}

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This study initially undertakes a detailed experimental two-dimensional analysis of vector fields in both structured and random porous media configurations. Structured media are examined at porosities of 55%, 75%, and 85%, while random media are analysed at 75% porosity. As shown in Figure 1, both the axial and transverse velocity fields are significantly influenced by the geometry of the porous material, despite having the same porosity. This demonstrates that the pore arrangement at the interface profoundly impacts the flow behaviour at the boundary between the two domains. The more structured the pore configuration, the more the flow aligns axially, resulting in higher slip velocities. A detailed study is then dedicated to the analysis of the domain at the mesoscale. To develop appropriate tools for identifying this scale, a thorough analysis is performed to determine the optimal size of the representative elementary volume (REV) for studying the system, as reported by Figure 2. For systems with well-structured porous materials, the REV scale exhibits geometric characteristics, where the optimal length associated with the unit volume is $l_{opt} \approx l_t + l_p$. In contrast, for systems with random porous materials, a method based on a deviation tolerance is employed. The study highlights the critical impact of inadequately calibrated REV scales on the accuracy of experimentally derived coefficients, such as the Beaver and Joseph slip velocity coefficient and the Whitaker stress jump coefficient. It demonstrates that improper calibration leads to significant inaccuracies, rendering these coefficients unreliable for practical applications and theoretical modelling. To address this issue, the research concludes with the development of an analytical model grounded in a single-domain approach, employing the Darcy-Brinkman framework to describe the axial component of the coupled system. Particular attention is given to the interface at the mesoscale, where the coupling between free-flow and porous regions is most pronounced. This model provides a refined and consistent representation of flow dynamics across the interface, offering improved reliability for macroscopic modelling and a deeper understanding of the mesoscale phenomena that govern flow behaviour in coupled systems for microfluidic applications.

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Poster / 279

Coupling an immersed boundary method with local front reconstruction for modeling highly accurate contact line dynamics

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Multiphase flows in the presence of complex solid geometries are omnipresent in porous media processes. Resolving the associated phenomena on a pore level requires the accurate capturing of capillary forces, contact line dynamics and viscous resistance. Frequently, front capturing methods are used to present fluid-fluid interactions, i.e. the Volume of Fluid method (VoF). There, the accuracy depends on the reconstruction of the interface from an indicator function, effectively requiring a high resolution to meet common accuracy requirements and special treatment for multiphysics modeling.

As an alternative we implemented three- phase contact line dynamics for the front tracking method Local Front Reconstruction Method (LFRM) [1]. The fluid-solid interactions are accounted for by enforcing the no-slip boundary condition at the solid surface, which is done using a second-order implicit Immersed Boundary Method (IBM) [2]. Coupling of these methods consists of dynamically enforcing the local contact angle of the fluid-fluid interface with the solid surface. Additionally, the existence of a sharp interface allows for a high local control of the application of additional transport phenomena.

Here we describe the numerical model that is used to manipulate the fluid-fluid interface to enforce the local contact angle and assess its performance using droplet spreading simulations on flat and spherical surfaces. The equilibrium droplet shape (i.e. the radius, height and interface outline), interfacial pressure difference, surface tension force and spurious currents are compared to analytical solutions and literature standard front capturing methods. The results show an excellent match with the analytical solutions with error margins below 1% for the interfacial shape and pressure difference of almost all cases, as well as error norms in the order of 0.01% for the surface tension force and spurious currents. These error values are lower than for state-of-the-art front capturing models [3,4]. Furthermore, the model is extended with a coupling to discrete surface meshes, e.g. provided in the STL format. With this additional functionality, the model provides a pathway for modeling interface dynamics in complex geometries and a platform for further coupling with transport phenomena.

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MS07 / 280

Modeling processes in the Arctic from pore- to Darcy scale

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The Arctic is a complex and vast environment studied by many interdisciplinary teams. In the talk we present our recent results on modeling coupled thermal, hydrological, and mechanical processes in porous soils as well as in the snow portions of the cryosphere. While many models exist for these processes in other contexts, the special features of the Arctic including the subfreezing temperatures, substantial influence of the atmospheric controls, and paucity of data make the modeling from first principles quite valuable, since any model results are hard to verify.

In the talk we present our recent modeling results from first principles at the pore-scale up to the Darcy scale of these coupled processes in the Arctic.

In particular, we account for the change of constitutive properties associated with the freezing/thawing phase transformation in nano- to micro- to meso- and to macro-pores, which result in the liquid water fraction being a continuous rather than a discrete graph known from the Stefan problem. The theoretical and computational derivations we pursue for the upscaling from pore- to the Darcy scale turn out to produce upscaled constitutive properties close to the empirical relationships including the well known Soil Freezing Curve.

Furthermore, the flexibility of working with both of the two scales from the first principles helps to unify the thermal model for soils with the thermal conduction model for the snow, and makes it easy to couple these together. We are also able to account for the flow and deformation coupled to the thermal processes, and to calculate the Darcy scale properties such as the permeabilities depending on the presence of ice at the pore-scale.

This is joint research with Lisa Bigler, Naren Vohra, Zachary Hilliard, Praveeni Mathangadeera, Madison Phelps, and with other students and collaborators to be named in the talk.

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MS03 / 281

Fracture displacement basis function method for fast geomechanical simulations of fractured rocks

Authors: Giulia Conti¹; Stephan Matthai²; Patrick Jenny^{None}

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Predicting what permeability enhancements are feasible in a geothermal system (EGS) and the potential seismic activity they may trigger is challenging. Geomechanical simulations are computationally expensive because they require a discretized fracture network with a relevant level of complexity and a quantification of frictional sliding and tensile opening of individual fractures therein. Yet, computations of the fracture aperture distribution are essential, because they are decisive for predictive simulations of coupled flow and transport in EGS.

Here, we model this deformation assuming that the rock matrix is homogeneous with linear elastic behavior and that the slip profile of failing isolated fractures is elliptic with a linear relationship between maximum slip and induced stress. We employ such simplified single-fracture slip solutions as basis functions to predict displacement fields. Overall stresses are obtained by mapping the basis functions to the fracture ensemble of interest. This stress field combines far-field- and all slip-induced stresses, constraining the maximum slip and tensile opening along each fracture while considering local force balance constraints.

We illustrate the method for single-, parallel-, and intersecting fractures, as well as fracture networks. Importantly, our approach dramatically reduces the number of degrees of freedom as compared to an element-based mechanics simulation of the same model. It also permits the calculation of displacement and stress fields via superposition of precalculated basis functions. This opens the door to coupled mechanics, flow and transport in realistic EGS.

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Diffusive mixing between hydrogen and cushion gas: Implications for underground hydrogen storage

Authors: Yuhang Wang¹; Li Rong¹; Zhe Wang¹; Huirong Guo¹; Wanjun Lu¹

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The diffusive process between H₂ and cushion gas affects the purity of H₂ stored in the subsurface porous media. It is essential to understand the diffusive mass transfer and its impact on the migration of H₂. CO₂, CH₄, and N₂ serve as promising options for cushion gas. However, due

to experimental challenges, there has been limited research conducted to quantify the diffusion between H₂ and these gases under reservoir conditions. In this study, we present the first quantitative measurements of the diffusive process between the binary system composed of H₂ and the cushion gas in a high-pressure optical cell. Raman spectroscopy was used to monitor the diffusive process in real-time, and the diffusion coefficients were determined from the measured concentration profiles. We showed that the Fick's second law with a constant diffusion coefficient adequately describes the observed diffusive process. Correlations were then proposed to predict the diffusion coefficient for each cushion gas. Notably, the diffusion coefficient for CO₂ scales linearly with the reciprocal viscosity of CO₂, while for CH₄ and N₂, the diffusion coefficient is influenced by both the temperature and density of the cushion gas. Using the measured diffusion coefficients, we estimated the diffusion distances within reservoir rocks at field-scale. Results suggest that the dispersive mixing plays a role in the purity of the produced H₂.

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MS10 / 284

A novel 4D X-ray micro-particle velocimetry approach: enabling faster measurements in porous media

Author: Robert van der Merwe¹

Co-authors: Wannes Goethals¹; Sharon Ellman²; Sojwal Manoorkar¹; Jan Aelterman³; Matthieu Boone⁴; Tom Bultreys¹

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Fluid flows in porous media play a crucial role in both natural and industrial processes, such as underground hydrogen storage for renewable energy and water-gas management in fuel cells. Intricate pore geometries drive complex, multi-scale dynamics in phenomena such as multiphase and viscoelastic flows. Accurate modeling of these flows is challenging however, as numerical simulations are computationally intensive and limited by physical uncertainties. Particle velocimetry methods, particularly Lagrangian particle tracking (LPT), enable direct measurement of complex flow patterns near pore walls using representative tracer particles, but require transparent geometries for conventional optical methods.

The penetrating power of X-rays, combined with computed tomography methods, enables non-invasive probing of internal dynamics in opaque materials. By acquiring X-ray projection images from many viewing angles, high-resolution 3D reconstructions of a sample's interior can be generated over time, enabling the direct tracking of tracer microparticles. This approach was first demonstrated for creeping flows in opaque porous media using silver-coated hollow glass tracers (Bultreys

et al., 2022) and has since provided new insights into complex 3D phenomena, such as Haines jumps in multiphase flow (Bultreys et al., 2024). Despite these advancements, the temporal resolution of 3D tomography remains constrained by long acquisition times relative to the timescales of many pore-scale flow dynamics (commonly ms to s). Consequently, artifacts produced by particle motion degrade tracking capabilities for velocities exceeding 1 $\mu\text{m/s}$, confining the method to slower and less complex flow regimes.

We address this limitation through the development of a novel tomographic reconstruction algorithm, adapting elements of current state-of-the-art LPT methods (Schanz et al., 2016). Additionally, we optimize data processing workflows and experimental setups by refining hardware, imaging settings and tracer particle selection. Our goal is to improve particle tracking time resolution while maintaining micrometer-scale measurement capabilities. We present proof-of-concept results applied to both simulated and experimentally measured datasets on slow, simple flows. These developments aim at extending the method's applicability to fast, unsteady 3D flows, requiring increasingly complex validation to ensure robust performance.

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285

Drying at high heating rate in porous media: Application to biomass pyrolysis

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The present study investigates the impact of high heating rates on the drying behavior of porous media, focusing on the characterization of the physical phenomena occurring at the pore scale.

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MS08 / 287

Visualization and characterization of spreading and mixing at the pore-scale relevant for Geological Carbon Sequestration and Underground Hydrogen Storage

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Geological Carbon Sequestration and Underground Hydrogen Storage in porous reservoirs are promising strategies for transitioning to clean energy production. Gas dissolution in brine significantly influences flow and trapping behavior during both CO₂ and H₂ storage in porous reservoirs. Interestingly, for H₂ storage, this effect was unexpected due to hydrogen's low solubility in brine. However, recent experiments have revealed rapid dissolved H₂ transport that is not captured by current state-of-the-art models. To better understand the transport behavior of dissolved gasses in these systems, we conduct steady-state single-phase microfluidic experiments to visualize spreading and mixing at the pore scale. The experiments are carried out using two microfluidic chips with homogeneous and heterogeneous pore structures, each containing two inlets and two outlets. A pH indicator solution saturated with the gas is injected at one inlet, while a pH indicator solution without any dissolved gas is injected at the other, forming a mixing zone along the chip's center line (figure 1). The color change of the pH indicator solution reveals variations in dissolved gas concentration, visualizing the spreading and mixing of the dissolved gas. Experiments are conducted for both H₂ and CO₂ at atmospheric pressure and room temperature conditions across eight flow rates, covering advection- and diffusion-dominated transport regimes. The experimental results are compared to direct numerical simulation using the *interReactiveTransferFoam* module of the GeoChemFoam [1](#) solver package. Here the species transport of dissolved H₂ and CO₂ are solved with constant flow inlet and constant pressure outlet boundary conditions.

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References:

[1](#) DOI:10.5281/zenodo.11354428

MS01 / 288

Quantification for density-driven convection of CO₂ in water

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Given the growing concerns about climate change, reducing anthropogenic carbon accumulation in the atmosphere has become a critical focus. Carbon capture and storage (CCUS) has gained increasing attention as an effective midterm measure that could accommodate massive amounts of CO₂ underground (32 gigatons per year)[1,2]. As one of the important mechanisms of CCUS, solubility trapping greatly determines the efficiency of CO₂ sequestration. The carbon dissolution rate largely depends on the density-driven convection (DDC) of CO₂ in water. Various factors are deciding the CO₂ convection behavior in the porous media[3], making it challenging to interpret. Although there are multiple relevant simulation works, experimental studies are still lacking in quantifying the phenomena. The opaqueness and uncertainty of most porous media complicate the reproduction of experimental results and the quantification of DDC. In our experimental study, we primarily employed optical 3D-printed porous media with defined pore structures and properties to conduct carbon convection experiments. To visualize the CO₂ convection patterns under different experimental conditions, we utilized a novel universal pH indicator that covers a broader measurable pH range (4.4 to 9.6) and detects subtle pH variation (below 0.1 pH unit)[4]. By mapping the colors of indicators to the pH, we can determine the spatiotemporal pH and total dissolved carbon, which quantitatively indicates the CO₂ convection. Our error analysis indicates that our experimental techniques have a smaller margin of error in carbon measurement compared to previous studies[2,5]. Furthermore, we quantified the convection behavior by determining the mixing length, carbon flux across the interface, and the wavenumber, etc[6,7]. This experimental work can be of great interest to CCUS projects.

Keywords: Carbon capture and storage, density-driven convection, experimental techniques, quantification

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MS06-A / 289

The microscale dynamics of water films during evaporative precipitation of minerals in porous media

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Wetting and drying cycles are often found in natural and engineered porous medium exposed to water. Examples include soils, underground porous rocks or building materials. When a porous medium dries, minerals contained in the water can supersaturate and consequently precipitate. The location and mechanism of precipitation of these minerals is dependent on the drying dynamics, which are controlled by the atmospheric conditions (e.g. humidity/temperature) as well as the structure and chemistry of the porous medium (and the evolution of structure and chemistry during the process). In hydrophilic media, connected water films are often retained on the pore surfaces during evaporation. These films can contribute to the drying rate by allowing water to flow through them towards the evaporation front. This leads to supersaturation at the outer surface of the porous medium, resulting in nucleation and growth of precipitates at the outer surface, a process known as efflorescence. The precipitates that form are often porous themselves and can contain water films which supply supersaturated water that can sustain their growth [1]. Efflorescence often occurs in building materials exposed to wetting and drying cycles of rainwater, but a similar phenomenon also can occur in porous reservoirs when they are used for injection of a dry gas such as CO₂ or hydrogen.

The effects of structural properties of the porous medium, such as the pore surface roughness, on how the drying process and efflorescence formation take place are still a large open question. In this study, we focus on the dynamics of the water film on the outer surface of the porous medium, by imaging the mineral nucleation and growth from water films and investigating how the surface structure plays a role in the initial phases of precipitation. We developed a technique for measuring dynamics of water films and surface structure evolution using in-situ atomic force microscopy (AFM) on the grains of a porous limestone [2], which we saturated with NaCl solution. This allows us to track the water film and precipitate formation on the surface during the entire drying period. The measurements show that the film decreases in size in a non-uniform way largely dependent on the initial surface structure. Precipitates predominantly form inside cavities in the surface topology, indicating a significant effect of surface structure. The insights from this study are valuable as input for drying models taking into account film dynamics and surface structure.

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Poster / 290

Advancing Pore-Scale Measurements: Enhancing Curvature and Contact Angle Analysis for Immiscible Two-Phase Flows in Porous Media

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Conducting coreflooding experiments with high-resolution imaging has become a key approach for understanding the physical phenomena governing CO₂ storage in underground porous geological formations. These experiments focus on displacement and trapping mechanisms of immiscible phases, which are predominantly capillary-dominated. A significant advantage of pore-scale imaging lies in its ability to capture the interface between any two phases, enabling the in-situ measurement of contact angles and curvature (capillary pressure). These measurements are crucial for quantifying how rock heterogeneity influences flow, as capillary forces are governed by wettability and pore space structure. Contact angles also serve as vital input parameters for pore-scale simulations, where pore-by-pore contact angles dictate the sequence of pore displacement. Additionally, experimental capillary pressure measurements validate the predictive capabilities of simulations.

However, both contact angle and curvature measurements are highly sensitive to image processing methods. Current approaches often derive these properties from segmented images, which are prone to high error rates. Segmentation methods eliminate intensity gradients that indicate phase transitions (interface boundary), leading to the loss of critical features needed to preserve the true geometry of interface boundaries. Furthermore, when interfaces are extracted on discrete surfaces with stair-step geometries, smoothing operations intended to improve surface quality can inadvertently introduce curvature errors. Even minor errors can significantly amplify the margin of error for contact angle measurements.

This study addresses these challenges by developing automatic, open-source tools to improve curvature and contact angle measurements. The approach enhances the extracted interface surface between phases by leveraging sharp intensity gradients from grayscale images. A neural network is trained to recognize interface geometries under various wetting conditions, such as minimal surfaces, concave menisci, and convex menisci. Training is conducted using synthetic images with analytically known curvatures and real two-phase flow images from rock samples. The tools also refine geometric contact angle measurements by analyzing three-phase loops (fluid-gas-solid contact regions) and extracting angles based on localized interface geometry, rather than relying solely on contact node information. By advancing these methodologies, this study improves the accuracy and reliability of key pore-scale measurements, providing more robust data for simulations and enhancing our understanding of multiphase flow in geological storage systems.

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Electrical Monitoring of Foam Propagation in Porous Media: Spectral Induced Polarization (SIP) and Time Domain Reflectometry (TDR) Measurements in a 2D Tank

Author: Abbas Shoker¹

Co-authors: Alexis Maineult²; Azita Ahmadi-Sénichault³; Dorian Davarzani¹; Fabien Lion¹; Jacques Deparis¹; Julia Holzhauser¹; Pauline Kessouri¹; Philippe Leroy¹; Stefan Colombano¹

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Monitoring subsurface processes during soil remediation is crucial for optimizing environmental restoration techniques. Geophysical tools, such as Spectral Induced Polarization (SIP) and Time Domain Reflectometry (TDR), offer non-invasive methods for tracking these processes. This study focuses on the electrical monitoring of foam propagation in saturated porous media to enhance remediation strategies for hydrocarbon-polluted aquifers.

Aqueous foam, consisting of gas bubbles dispersed in a liquid phase containing surfactants, is widely used in soil remediation due to its high viscosity and its ability to act as a blocking, mobilizing, or vectorizing agent. Understanding the electrical properties of foam propagation is essential for evaluating the effectiveness of the use of electrical methods for monitoring foam flow in remediation processes.

Our experiments were conducted in a 2D tank packed with 1 mm glass beads and saturated with tap water (400 $\mu\text{S}/\text{cm}$) Figure 1. The foam was generated using an anionic surfactant (SDS) and injected into the tank at a gas fraction (foam quality) of 85% and a constant flow rate of 8 mL/min. The SIP method was employed to measure complex electrical resistivity across frequencies ranging from 1.46 Hz to 187 Hz, while the TDR method was used to assess relative permittivity and electrical conductivity at the frequency of 70 MHz. Additionally, image monitoring was utilized to convert optical densities into foam saturation values (Sf), providing a means to validate the geophysical measurements.

The results, (Figure 1, Figure 2), show that foam propagation causes significant changes in dielectric permittivity and resistivity in regions affected by foam injection. For the central zone, Probe 13, the dielectric permittivity decreases by 63% (from ~19 to ~7), while resistivity increases up to 6000% (~85 $\Omega\cdot\text{m}$ to ~5100 $\Omega\cdot\text{m}$). In contrast, Near-Center zones, e.g. probe 12, show moderate changes (~33% permittivity decrease, ~120% resistivity increase). Probes in the edge zones, such as Probe 11, show no significant changes in permittivity or resistivity, as the foam propagation did not reach these areas. This lack of variation validates that foam impact is confined to the central and intermediate zones. The observed foam saturation from image analysis validates the geophysical measurements, with higher foam saturation (up to 90%) in the central zone correlating with greater electrical property changes. Additionally, we observe higher phase shifts in Probe 13, Figure 3. We are further analyzing the phase-frequency variation (1.46 Hz to 20 kHz) to better understand the polarization effects induced by foam.

These findings highlight the potential of SIP and TDR methods for monitoring foam flow in porous

media and provide valuable insights into the complex interactions between foam and electrical properties. This study underscores the importance of integrating geophysical techniques with image-based analysis to improve the understanding and effectiveness of soil remediation processes.

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Cotransport behavior of zinc oxide and copper oxide nanoparticles in soil

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Zinc oxide (nZnO) and copper oxide (nCuO) nanoparticles are among the most widely used nanoparticles. They enter the subsurface through various sources such as industrial effluents, sewage, and agricultural activities, leading to groundwater contamination. This study investigated the cotransport behavior of nZnO and nCuO in saturated soil through column experiments and mathematical modeling. We observed decreased transport of both nZnO and nCuO during their cotransport as compared to their individual transport. This is due to the formation of large-sized heteroaggregates which have a greater retention in soil than free nZnO and nCuO. Further, nCuO transport was retarded to a greater extent than nZnO. This is due to the greater affinity of nCuO than nZnO to attach to the grain surfaces and the greater mass fraction of nCuO than nZnO in the heteroaggregates. The experimental results were successfully simulated using a mathematical model which accounted for nZnO and nCuO retention in soil, kinetics of heteroaggregation, and heteroaggregate retention in soil.

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Effect of soil biofilms on the transport of ZnO nanoparticles

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Increasing production and wide application of zinc oxide nanoparticles (nZnO) lead to their ultimate release into the environment and cause soil and groundwater contamination. Attached bacteria are ubiquitous in the subsurface and can affect the transport of nZnO. This study investigates the influence of soil biofilms on the fate and transport of nZnO through a coupled experimental and modelling approach. nZnO transport reduced significantly in the presence of biofilm. The experimental results were successfully simulated using a dual-porosity model, which accounted for nZnO transport and retention and nZnO mass exchange between soil and biofilm.

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Water & Porous Media Focused Abstracts:

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- [3] Delay, F., Porel, G., & Chatelier, M. (2013). A dual flowing continuum approach to model denitrification experiments in porous media colonized by biofilms. *Journal of contaminant hydrology*, 150, 12-24.

Poster / 298

Adsorption and diffusion of shale gas in nanopores with different mineral cleavage surfaces: Insights from density functional theory and molecular simulations

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Shale gas has begun to progressively replace traditional oil and natural gas as a new significant energy source due to the gradual advancement of shale gas exploration and development technology. Exploration and extraction of shale gas depend on the adsorption and free-state characterization of gases in nanoporous shale. Although the majority of current research focuses mostly on the traditional solvation surface of minerals, shale minerals feature a variety of intricate surface and adsorption micro-mechanisms. Thus, using DFT (Density Functional Theory), this work first optimizes and analyzes the significant cleavage surfaces of quartz, calcite, feldspar, and illite and evaluates the major cleavage surface attributes based on the XRD data of genuine shale. According to the simulation results, all four of the outermost exposed atoms of minerals in their most stable states are oxygen atoms, and the arrangement of these atoms varies depending on the kind and disintegration direction of the mineral. Furthermore, the adsorption and diffusion behaviors of gases like methane and carbon dioxide in nanopores made from the typical solvation surfaces of various minerals were examined using molecular dynamics simulations. The findings demonstrate that, in the nanopores of the same mineral with distinct disintegration surfaces, the adsorption and diffusion behaviors of gases varied significantly. In the meantime, the quantity of oxygen atoms exposed on the surface is directly correlated with the adsorption of methane and carbon dioxide in nanopores. The present investigation serves as a theoretical manual for the exploration and recovery augmentation of shale gas reserves from the standpoint of gas adsorption.

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MS06-A / 300

Cross-scale investigation of coupled mineral dissolution and precipitation with gas exsolution in porous media

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Coupled mineral dissolution, precipitation, and gas exsolution are critical in subsurface energy applications such as natural hydrogen extraction, nuclear waste storage, and CO₂ sequestration. However, the behavior of exsolved gases in rock matrices remains poorly understood, particularly regarding whether gases become trapped by precipitates, induce pore clogging, or migrate with fluid flow and dissolve downstream. These uncertainties hinder the accuracy of reactive transport models for long-term predictions. To address this, we conducted microfluidic experiments using a model system based on witherite dissolution, barite precipitation, and CO₂ exsolution to identify the conditions under which gas is produced and their in these systems. Microfluidic experiments, combined with in situ Raman spectroscopy and geochemical modeling, revealed that CO₂ bubbles formed during dissolution serve as nucleation sites for barite. CO₂ bubbles became enclosed by precipitates when the barite crystallization rate exceeded the CO₂ production rate, a process controlled by the acidity of the solution and the solution's saturation with respect to barite. These were followed by core-scale experiments to investigate whether the gases produced during the reactions are trapped

or transported in the porous media. Magnetic Resonance Imaging (MRI) was used to monitor heterogeneous gas production, transport, and relative gas content in porous media over time. These results were complemented by measurements of pH, pCO₂, differential pressure, and effluent ion concentrations. Scanning electron microscopy showed porosity reduction due to barite precipitation and localized clogging at bubble surfaces. Our experiments highlight key areas requiring further investigation, as current empirical models like Van Genuchten-Mualem and Brooks-Corey fail to account for chemical reactions that alter pore geometry, connectivity, and wettability. While reactive transport modeling addresses multi-phase flows and mineral reactions, existing codes like TOUGHREACT and PFLOTRAN lack the ability to fully couple precipitation, dissolution, and gas dynamics. Advanced mathematical coupling approaches and refined porosity-permeability models are essential for accurately simulating the interplay of these processes, especially under conditions involving gas generation and transport.

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References:

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Microscopic Simulation and Characterization of Transport and Bridging Behaviors of Colloidal Particles in Gravity-packed Beads

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Investigating colloidal particles' transport and deposition mechanisms in porous media holds significant academic value for numerous scientific and engineering fields. To gain an in-depth understanding of colloidal particle deposition in porous media, a two-way coupling computational fluid dynamics-discrete element method (CFD-DEM) approach was developed, which was well validated by the classical Kozeny-Carman equation. We conducted numerical simulations on the transport and deposition of colloidal particles with different sizes in randomly packed beads, and observed the particle transport and bridging phenomena in single-phase water. The results show that the macroscopic deposition amount of particles exhibits a consistent growth trend over time, which can be well described by an S-shaped growth curve. Moreover, particle size has a significant influence on the deposition amount, leading to distinct quantitative trends and criticality in its temporal variation. To identify the microscopic mechanisms underlying this phenomenon, we compared the transport velocity and the trapping time probability density of particles with different sizes in porous media and revealed the relationship between particle size and the reversibility of deposition. This work provides a universal law and valuable insights for the quantitative description of particle deposition phenomena in porous media.

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MS06-B / 303

Modeling the foam dynamics in heterogeneous porous media

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Foam flow in porous media is important in various engineering applications, including soil remediation, carbon dioxide sequestration, and enhanced oil recovery. This study explores the relationship between bubble density and permeability in foam flow models, focusing on how different approaches capture foam formation in highly permeable regions. We compare two mechanistic models numerically. The first one is a Newtonian model with simple foam generation mechanics, while the second is a non-Newtonian model that incorporates complex mechanisms of foam generation and destruction depending on phase velocities and capillary pressure. Our results demonstrated that the more complex model exhibited a strong correlation between bubble density and permeability, while the simpler model maintained a constant bubble density despite the heterogeneity. While experimentally documented, this observed correlation was not analyzed from a theoretical modeling perspective. We developed a workflow for fitting the corresponding parameters based on foam equilibrium to compare both models.

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[1](#) JB Cedro, FF de Paula, G Chapiro, *Advances in Water Resources*, 104882, 2025 [2] FF de Paula, I Igreja, TO Quinelato, G Chapiro, *Advances in Water Resources* 188, 104690, 2024

MS06-A / 306

Preferential flow of dispersed fluid through doublet system

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Dispersed fluids (foam, emulsion, bubbly liquid, etc.) flows through porous media in the form of disconnected droplets or ganglia, which occurs in many subsurface industrial scenarios [1-3]. However, current theoretical models cannot provide a consistent and general description of the dispersed fluids flow in porous media [4,5].

We conducted demonstrative microfluidic experiments on dispersed blobs in a porous medium model. We varied Ca_d (dispersed fluid capillary number) and Ca (total capillary number), and the micro-model was homogeneous. Surprisingly, we observed significant non-uniform flow as shown in Fig. 1a. Preferential paths carry almost all the dispersed fluid flux, while blobs in other paths flow only occasionally and slowly. We observed similar preferential flow in a simplified doublet system (Fig. 1a). This phenomenon raises the question of whether it is caused by manufacturing errors or arises inherently.

We formulated a generalized model for the pressure drop F in a single channel, expressed as $F=f(Ca, S_d)$ (S_d , dispersed fluid saturation). We then conducted numerical simulations in a doublet system. When residual saturation (S_r) is absent as in classic straight-tube models [6], the droplet flux is equal in both channels. However, when we incorporate S_r to match the physics in porous media [7], a small geometric difference may lead to significant discrepancy in droplet flux at low Ca (Fig. 1b). This asymmetry is suppressed by increasing Ca (Fig. 1b). We theoretically rationalize this observation that highlights the role of residual saturation on breaking the symmetry. Further experiments successfully reproduce this theoretical prediction in a dual-channel system (Fig. 1c). These results demonstrate that manufacturing errors are not the primary cause of preferential flow.

In summary, microfluidic experiments and theory demonstrate that minor geometric differences in dual-channel systems can result in significant differences in dispersed fluids flux. This amplification of geometric asymmetry in flow asymmetry is a result of capillary trapping in the porous structure.

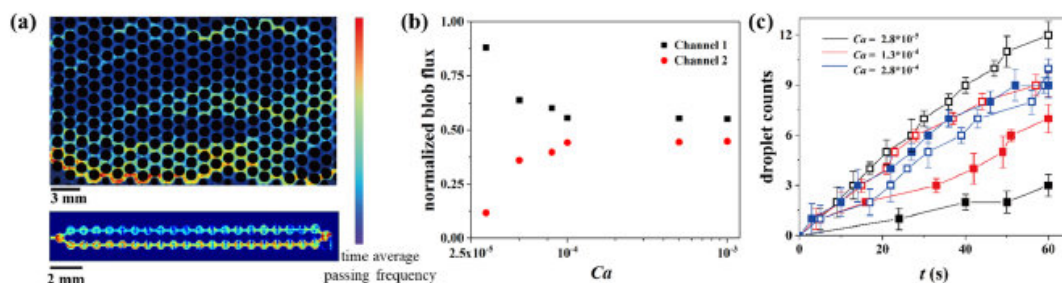


Figure 2: (a) Time-averaged blob-passing frequency field map of the porous media model and dual-channel system, where preferential paths are clearly identifiable. (b) Theoretical calculation results of blob flux as a function of the total capillary number Ca in the dual-channel system for $Ca_d = 1.5 \times 10^{-5}$. The black symbols represent the results for channel 1, while the red symbols represent the results for channel 2. (c) Experimental results of the cumulative number of droplets in the dual-channel system as a function of time for $Ca_d = 1.5 \times 10^{-5}$. Hollow symbols represent results for channel 1, while solid symbols represent results for channel 2.

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MS04 / 307

Pore Structure Evolution in Clays Under Drying and Wetting Cycles: Insights from Mercury Intrusion Porosimetry

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The evolving pore structure in soil, influenced by various physico-chemical activities such as erosion, climate change, mechanical loading, and chemical weathering, can lead to catastrophic events like landslides and slope failures. One significant factor contributing to pore structure changes in soil is the cyclic drying and wetting process, which profoundly impacts various soil properties. Clayey soil minerals, particularly kaolinite and bentonite, play a crucial role in these failures. The evolving pore structure of these clayey soils under varying environmental conditions, such as drying and wetting cycles, significantly influences their permeability, strength, and overall hydro-mechanical behavior. However, experimentally capturing this pore evolution is challenging due to various microstructural disturbances associated with different experiments. This study discusses an experimental protocol that employs Mercury Intrusion Porosimetry (MIP) to quantify the pore structure evolution of kaolinite- and bentonite-rich soils. The rearrangement of soil particles due to drying and wetting cycles may lead to clogging or alterations in pore shape, particularly in smaller pores, thus reducing their connectivity. These smaller pores are particularly crucial for water retention, so any structural changes can influence the soil's ability to hold and transmit moisture, impacting its hydraulic properties. Conversely, larger pores may collapse during drying, reducing their capacity to hold water. This study analyzes the pore sizes of kaolinite and bentonite soils under various drying and wetting cycles using MIP and Scanning Electron Microscopy (SEM). Since the oven-drying method relies on evaporation and can cause alterations in pore structure, the freeze-drying procedure is preferred to preserve the natural pore structure. This study also includes a comparative analysis of pore structure changes induced by oven-drying and freeze-drying methods. A pore structure evolution model (Equation 1), proposed by Li et al. (2023), has been adopted to evaluate the evolution of pore structure under different drying and wetting cycles. The bimodal pore size distribution function (PSD) at the final state, $f\log(d)$ is utilized to model the pore size distribution derived from MIP results.

Equation 1

The evolution parameter, calibrated using the PSD, provides insight into how the pore structure changes during the drying and wetting processes.

Figure 1a,b

The SEM image in Figure 1(a) shows the microstructural features of freeze-dried Bentonite soil, revealing intricate pore networks and particle arrangements. The freeze-drying process preserves the natural pore structure, minimizing collapse or alteration caused by water removal. Figure 1(b) illustrates the PSD of bentonite soil, comparing freeze-dried (FD) and oven-dried (OD) samples at 46% water content using MIP. The PSD curve indicates that the freeze-dried sample exhibits a higher proportion of smaller pores, while the oven-dried sample shows a shift towards larger pores, reflecting structural changes due to thermal drying. These observations underscore the significant impact of drying methods on pore structure, with potential implications for soil-water interactions and retention behaviour.

Reference:

K. Peng Li, Y. Gui Chen, W. Min Ye, and Q. Wang, "Modelling the evolution of dual-pore structure for compacted clays along hydro-mechanical paths," *Computers and Geotechnics* 157 (2023) 105308, <https://doi.org/10.1016/j.compgeo.2023.105308>

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References:**Poster / 308**

Current State of Exploring Dissolution and Precipitation Processes in Deep Geothermal Reservoirs of the Ruhr Area

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High-resolution X-ray Computed Tomography (XRCT) is a powerful tool for investigating phase differences in rock samples, such as pores and solids. Despite significant differences in bulk density or porosity between calcite and dolomite, their similar X-ray absorption coefficients lead to comparable gray-scale intensities, making phase differentiation challenging. Overcoming this limitation is essential for interpreting mineralogical transitions in geochemical experiments within a location-dependent volume.

This study addresses the challenge of visualizing and segmenting calcite and dolomite phase differences under hydrothermal experimental conditions by combining high-resolution XRCT and spectral tomography.

Dolomitization was replicated in laboratory conditions using hydrothermal reactors at 200°C with a Mg- and Zn-enriched reactive fluid. The fluid composition included MgCl₂, CaCl₂, ZnCl₂, and

NaCl, mimicking natural hydrothermal environments. Samples were treated for two weeks in static conditions with a high fluid-to-rock ratio, ensuring the reaction was not fluid-limited. Conventional XRCT workflows, which record the total intensity of the incident beam, were unable to differentiate calcite and dolomite due to their similar absorption properties. By integrating spectral tomography, which detects the energy of each photon separately, we were able to overcome these limitations and achieve clear differentiation between the two phases.

Using the combined approach of high-resolution XRCT and spectral tomography, we successfully distinguished phase differences between calcite and dolomite, which were undetectable with standard imaging methods. This approach enabled visualization of subtle mineralogical changes induced by hydrothermal treatment.

The successful application of this combined workflow results in the current state of sophisticated multiphase segmentation in four different reservoir rocks, enabling the evaluation of changes in key physical properties—such as elastic, hydraulic, thermal, and electrical properties—during hydrothermal experiments.

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 101005611 for Transnational Access conducted at DMEX-UPPA-FRANCE.

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MS01 / 309

CO₂ Mass Transfer in Porous Media: Implications for Long-Term Carbon Sequestration in Saline Aquifers

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A critical aspect of carbon sequestration involves understanding the transport and trapping mechanisms that influence the long-term stability of injected CO₂. Among these, solubility trapping, driven by the diffusion and convection of CO₂ in the aqueous phase, plays a pivotal role in enhancing the sequestration security of saline aquifers. This study investigates the dissolution of CO₂ in aqueous solutions within porous media using transmitted light visualization techniques. Experiments were conducted over a period of at least 96 hours in a sealed visualization cell designed to ensure system stability and enable precise monitoring. The porous media consisted of capillary tubes filled with bulk water and water-saturated glass beads of specified grain sizes. These media were saturated with pH-sensitive solutions to enable visualization of chemical changes. To maintain constant system pressure, CO₂ was continuously supplied to the visualization cell, compensating for gas mass transfer into the aqueous phase. The inflow of CO₂ was rigorously monitored in real-time, ensuring accurate control of the process. As CO₂ dissolved into the aqueous phase, it formed an acidic solution, resulting in a measurable change in the color of the pH-sensitive solution. This colour change, indicative of pH variation, was continuously captured and analyzed to provide insights into the

dynamics of CO₂ dissolution and its interaction with the porous media. Our experimental methodology enabled a comprehensive analysis of CO₂ mass transfer dynamics under two distinct conditions: (1) diffusive mass transfer supported by natural convection and (2) diffusive mass transfer with density-driven convection suppressed. Key observations were made by measuring the velocity of the gas-liquid interface, which reflects diffusive mass transfer, and by characterizing natural convection through parameters such as the onset time of convection, mass flux, and flow dynamics. The study explored the influence of salinity (NaCl), gas contaminants (N₂), and the grain size of porous media on CO₂ dissolution behavior. Results revealed that as the average grain size of the porous medium decreases, natural convection has a diminishing role in enhancing the dissolution process compared to diffusion alone. Specifically, smaller grain sizes led to a delayed convection onset time, which in turn reduced the convection-driven mass flux. This highlights the critical role of pore-scale interactions in influencing convective dynamics. Salinity was found to significantly impact the onset time of convection, as it directly affects key parameters such as fluid density, effective molecular diffusivity (affected by pore size), and viscosity. Increased salinity delayed the onset of convection, altering the balance between diffusive and convective mass transfer mechanisms. Additionally, the presence of even small concentrations of N₂ as a gas contaminant adversely affected overall CO₂ dissolution rates, underscoring the importance of gas purity in mass transfer processes. This study presents a novel experimental approach based on light transmission techniques to investigate CO₂ mass transfer dynamics in aqueous solutions within porous media. The insights gained from this work are critical for evaluating the efficacy of solubility trapping, a key mechanism for the secure and long-term storage of CO₂ in geological formations.

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MS08 / 311

A numerical lamellae method based on flow maps

Authors: Daniel Dominguez-Vazquez¹; Tomás Aquino¹

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A hyperbolic description of the problem of solute transport using a deterministic and Lagrangian formulation that combines characteristics of the classical formulations based on the Fokker-Planck (FP) and Langevin equations is developed. This formulation is based on a Liouville master equation, whose hyperbolicity allows for tracing the concentrations along characteristic lines in the augmented phase space composed by solute particle locations and a set of (time-independent) random coefficients used to define a source term that introduces the noise added to the system, in lieu of (time-dependent) stochastic processes. This circumvents the use of stochastic calculus and eliminates the diffusive term of the master equation, at the expense of increasing the dimensionality of the joint probability density function (PDF) of solute particle locations. The characteristic lines define flow maps for the joint PDF and its support such that all one-point space-time statistical information to study mixing and dispersion respectively is contained in them. Therefore, diffusion is modeled with kinematics parametrically dependent on random coefficients. This approach can be combined with numerical algorithms to solve ordinary differential equations (ODEs), that are unaffected by

the Courant-Friedrichs-Lewy (CFL) stability condition, do not suffer from Gibbs oscillations, do not require (order-reducing) filtering and regularization techniques, and do not rely on standard Monte Carlo sampling. Because of these reasons this formulation offers more accuracy and a lower computational cost in comparison to Eulerian grid-based and Lagrangian particle tracking solvers. To find the proper noise term to add, we impose that averaging the Liouville equation over the coefficients must lead to the FP equation, which leads to a classical closure problem for the moments of the joint PDF. However, assuming a local linearization in concordance with the Ranz transform used in the lamellae description, a simple closure based on truncated central moments becomes exact and so does this hyperbolic description, which accounts for diffusion in all directions. In this talk, I will discuss the methodological advantages of using a hyperbolic description of mixing, and show how it can be used to construct a numerical lamellae method for arbitrarily shaped initial concentration profiles.

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Transport and Retention Behaviors of Suspended Colloidal Particles in Randomly Packed inhomogeneous porous media

Author: Yaoming Chen¹

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The transport of particles in porous media, encompassing mechanisms such as dispersion and straining, is critical to optimizing various engineering applications, including drug delivery, wastewater treatment, and the displacement of proppants in hydraulic fracturing. While previous numerical studies have significantly advanced our understanding of particle transport at the microscopic scale, these investigations have predominantly focused on homogeneous packed beds. Consequently, the impact of porous medium inhomogeneity has been largely overlooked. When the porous structure exhibits inhomogeneity, the applicability of conclusions drawn from homogeneous systems may become limited or invalid.

To bridge this knowledge gap and evaluate our hypothesis, we simulated the Lagrangian transport of 3-D spherical particles through a 3-D inhomogeneous porous network generated by a randomly sedimented, saturated, inhomogeneous packed beds, employing a computational fluid dynamics-discrete element method (CFD-DEM) approach. To account for the effects of porous medium inhomogeneity on particle transport, we generated packed beds with varying particle size distributions while maintaining a constant median particle size (d50). A two-way particle-fluid coupling algorithm was employed to capture the bidirectional interactions between particles and the fluid: the fluid flow influenced particle motion, and conversely, particles altered fluid streamlines.

Our results suggest that, compared to prior studies on homogeneous packed beds¹, the critical particle size that induces a significant reduction in permeability differs and is correlated with the median particle size of the bed. Moreover, the probability of particle clogging is not linearly dependent on

the degree of inhomogeneity of the porous medium, with a critical value observed. These findings provide valuable insights into the design of particle properties to achieve specific deposition and dispersion properties in porous media.

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References:

 Feng Q, Cha L, Dai C, et al. Effect of particle size and concentration on the migration behavior in porous media by coupling computational fluid dynamics and discrete element method[J]. Powder Technology, 2020, 360: 704-714.

MS10 / 313

Hysteresis and breakthrough of dynamic water flow in asphalt mixture

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Dynamic water pressure caused by tire loads accelerates the deterioration of asphalt pavements, leading to water damages and material failure. Understanding water flow dynamics within the voids of asphalt mixtures during cyclic loading is essential for improving pavement performance in rainy regions.

This study developed an in-situ dynamic water flow testing setup within a Fast CT scanning environment. The X-ray projection processing method is utilized to analyze water breakthrough with a temporal resolution of 40 ms. The water flow dynamics in asphalt mixtures were successfully visualized, highlighting the water saturation hysteresis loop under cyclic pressure and capturing rapid water breakthroughs in micro-voids.

The results show that the increasing water pressure drives water to pump into open voids and compress the trapped air. Conversely, as water pressure decreases, the compressed air expels the water. This process illustrates water transportation within asphalt mixtures under cyclic tire loading and unloading. The water saturation hysteresis loop, linked to dynamic water pressure, exhibits a clockwise rotation, reflecting differences in water flow during pressure increases and decreases. Water breakthrough frequently occurs during pressure escalation, requiring a starting pressure of 0.5 MPa and occurring within 520 ms. During pressure drops, reverse breakthrough occurs as compressed air expels water, requiring a starting pressure of 0.3 MPa.

This study introduces a method to quantify water flow dynamics in porous media with high temporal resolution, offering valuable insights for studying water flow dynamics and transient water flow analysis.

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MS26 / 314

Mapping CO₂ migration pathways in 3D heterogeneous sedimentary structures

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Carbon storage is being increasingly relied upon by governments to reach their net-zero obligations. Leakage through permeable pathways such as abandoned wells and faults is identified as a potential risk for successful CCS implementation. Storage failure presents risks of environmental impacts to water resources, atmospheric emissions and reduction to the value of carbon credits. Gas migration pathways can be highly complex, rendering detection and assessment of leaks at surface challenging. It is therefore critical to understand the pathways gas may take when migrating through the subsurface. As gas migrates from the source, viscous forces are reduced, and gas migration is dominated by gravity and capillary forces. Consequently, the capillary entry pressures of the medium are a major control on migration. Small-scale heterogeneity has been shown to impact plume migration in storage reservoirs (Jackson & Krevor, 2020; Li & Benson, 2015). In the shallow subsurface heterogeneities are known to cause lateral migration away from leaking wells, and create ‘hot-spot’ gas distributions, impacting surface flux as well as dissolution in groundwater (Calvert et al., 2024; Forde et al., 2019). These processes can occur at much finer scales than can typically be considered in continuum field-scale models.

A strong body of work has developed on the role of subscale heterogeneities in storage applications. We apply a similar lens to understand the impact of centimetre-scale heterogeneities on the migration of gas in the shallow subsurface. Following the methodology of Meckel et al. (2017), we generate 3D metre-scale realistic sedimentary structures with varied depositional and petrophysical characteristics. Neglecting viscous forces, we are able to apply macroscopic invasion percolation (MIP) to domains with much higher resolutions than are typically feasible (e.g., 10s of millions of elements) while accurately capturing the capillary dominated flow observed in gas migration studies. Given the computational efficiency of MIP, we are able to simulate thousands of gas injections at high resolutions, and analyse the ensemble of results. This talk will present findings from simulations of gas migration through multiple 3D sedimentary structures at the metre-scale to better understand the migration pathway controls in the shallow subsurface. These findings help to improve our understanding of gas source zones, and controls on vertical and lateral migration.

Country:

United Kingdom

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Student Awards:

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Impact of Dual Wettability on Two-Phase Flow Dynamics in Porous Media

Author: Fei Jiang^{None}

Co-authors: YAOTIAN GUO ; Takeshi Tsuji¹; Shinsuke Mochizuki²

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Natural porous media are typically composed of various minerals with distinct wettability characteristics, making it crucial to analyze the impact of wettability distributions on multiphase flow behavior. In this study, a three-dimensional digital rock model with mineral distributions was reconstructed from X-ray μ CT images of Boise sandstone by employing the gradient boosting decision trees (GBDT) machine learning method, trained using QEMSCAN images obtained from the same rock sample. For training, 2D QEMSCAN images were collected at different depths of the Boise sandstone core, and these were matched with μ CT images from corresponding depths. The trained model was then used to directly label the μ CT images, generating detailed mineral distribution data. The analysis identified quartz and albite as the primary components, accounting for 72% and 28% of the rock, respectively. Based on this composition, the digital rock model was simplified into a dual-wettability framework. Subsequently, a multiphase lattice Boltzmann (LB) model was employed to simulate two-phase flow within the dual-wettability digital rock model. The influence of dual wettability on the relative permeability curve, immiscible displacement dynamics, and capillary trapping (initial-residual saturation curve) was thoroughly examined. Additionally, an artificial bead pack porous model with varying degrees of wettability heterogeneity, quantified using a heterogeneity index, was generated. The multiphase flow simulations conducted on the bead pack model revealed that greater wettability heterogeneity resulted in a lower relative permeability for the wetting fluid and a diminished recovery efficiency for the nonwetting fluid.

Country:

Japan

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Student Awards:

Water & Porous Media Focused Abstracts:**References:**

MS06-B / 317

Boundaries regulates convection, dispersion and solid-liquid phase change in porous media under Rayleigh-Darcy convection**Author:** Ke Xu¹**Co-authors:** Yumin Wang ; Chenglong Hu ¹; Yantao Yang ¹¹ *Peking University***Corresponding Authors:** kexu1989@pku.edu.cn, 2101111993@stu.pku.edu.cn

Rayleigh-Darcy (R-D) convection emerges when fluid density at the top is higher than that at the bottom in a porous stratum. This density mismatch may be induced by geothermal gradient or concentration contrast during CO₂ or mineral dissolution. R-D convection largely determines the vertical heat and mass transfer, and may significantly reshape the porous matrix.

Here we introduce our recent experimental, numerical and theoretical works on some interesting phenomena correlated to interface and boundary effects during R-D convection. These works include:

- 1) Solid dissolution that induces R-D convection. When the porous matrix contains soluble components (such as ice in permafrost beneath salt water, carbonate in sandstone with acid environment, and oil sand reservoir under solvent extraction), we experimentally observe fingering dissolution interface at low Rayleigh number (Ra) and stable dissolution interface at high Ra. We theoretically rationalize this observation by the competition between horizontal dispersion and vertical circumflex, which controls the growth rate of interface perturbation.
- 2) Vertical transport efficiency with non-straight boundary. Vary few works discussed how non-straight boundary affect R-D convection. We conduct numerical simulations with one boundary a sine curve. As expected, wavy boundary regulates the large-scale convection envelope. However, this regulation of convection results in different modification of vertical transfer behaviors compared to that with straight boundary: when $Ra < 1300$, vertical transport efficiency is enhanced by the wavy boundary; when $Ra > 10000$, vertical transport efficiency is suppressed by the wavy boundary. We rationalizes these two regimes by the evolution of bottom stable stream under different Ra .
- 3) Horizontal dispersion coefficient of a passive scalar under R-D convection. We surprisingly observe that although convection keeps intensifying with Ra, horizontal dispersion coefficient scales with Ra only in a narrow regime, and keeps unchanged when $Ra > 2500$. We rationalize this two-stage dispersion coefficient variation: at low Ra, passive scalar migrates through stable bulk circumflex; at high Ra, boundary layer with dynamic micro-plumes becomes dominant horizontal transport channel. Dimensionless analysis reveals the dependence of ultimate dispersion coefficient with Lewis number and molecular diffusivity.

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China

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References:

MS15 / 319

Determination of effective transport parameters on high-resolved 3D microstructures using CNN

Authors: Rishabh Saxena¹; Thomas Carraro¹

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The microstructure of (composite) materials is essential in assessing their performance in applications such as fuel cells, hydrogen storage and batteries. High-resolution microstructural data plays a critical role in optimizing the properties and functionalities of these materials. However, conventional imaging methods, such as CT scanning and FIB-SEM, are sometimes limited by their high expense and time required. To overcome these restrictions, we propose a deep learning-based approach to generate high-resolution from low-resolution 3D microstructure images. We present a SRResNet, a convolutional neural network (CNN) that is specifically trained on low-resolution microstructure data and provides a cost-effective and efficient approach for super-resolution reconstruction.

The SRResNet represents a significant progress in super-resolution technology by extending deep learning applications from 2D to 3D microstructures. To assess the physical properties and functional behaviour of the super-resolved 3D microstructures, we present a thorough morphological investigation. Effective transport parameters are a major focus of this study since they are essential for understanding and optimizing material performance. Key transport parameters such as effective tortuosity and permeability are computed using Laplace and Stokes equations, respectively, via finite element methods (FEM).

Our results show that the SRResNet captures intricate details of microstructural features with high fidelity reflected in metrics such as PSNR, SSIM, and surface accuracy. This work highlights the potential of SRResNet as a promising tool for material design and optimization, contributing to advancements in energy and transportation technologies

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Germany

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Student Awards:

Water & Porous Media Focused Abstracts:

References:

MS12 / 320

Pore-scale Analysis of Carbonate Acidification Based on CT Scan Imaging: An Experimental Investigation

Author: Victoria Farçal Rocha da Costa¹

Co-author: Leonardo José do Nascimento Guimarães

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Well-stimulation techniques are designed to mitigate formation damage phenomena. Matrix acidizing, a standard stimulation method, involves injecting an acidic fluid into the formation near the well to dissolve rock matrix minerals, create dissolution channels, enhance permeability, and restore well flow. Hydrochloric acid (HCl) is the most commonly used acid for this purpose; however, its high reaction rate with carbonates can limit its penetration into the formation. To optimize acid usage and increase the depth of wormholes, it is crucial to develop stimulation fluids with additives that slow down the acid's dissolution of the rock matrix.

This study aimed to understand the impact of stimulation fluids on the rock's petrophysical and geomechanical properties. Computed microtomography (μ CT) was employed to analyze the resulting wormhole patterns. Key characterizations included reactive fluid properties, carbonate rock samples, porosity and permeability measurements, rock mechanics tests, porous media flow tests, and X-ray μ CT imaging.

The results revealed significant weakening and stiffness loss in the rock after acid treatment. Samples treated with 15% HCl exhibited Young's modulus values approximately 96% lower than those of the intact samples, while those treated with 15% HCl plus additives showed a 22% reduction. Conversely, the 15% HCl group displayed a Poisson's ratio 39% higher than the intact samples, compared to a 15% increase for the additive group. The uniaxial compressive strength (UCS) of the 15% HCl group was around 60% lower than that of the intact samples, whereas the additive group showed an 8% reduction. Similarly, diametral compressive strength for the 15% HCl-treated samples was approximately 17% of the UCS, while the additive-treated samples achieved about 8%.

Micro-computed tomography visually confirmed the creation of fluid flow pathways from the reservoir to the well due to acid treatment. Rock mechanics findings highlighted that samples treated with 15% HCl and additives suffered less damage to their rock matrix than those treated with 15% HCl alone.

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Brazil

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Optimization of Thermochemical Energy Storage Reactors Using Machine Learning

Author: Torben Prill¹

Co-authors: Marie Gollsch¹; Marc Philipp Linder¹; Thomas Jahnke¹

¹ German Aerospace Center (DLR)

Corresponding Authors: torben.prill@gmx.de, marc.linder@dlr.de, marie.gollsch@dlr.de, thomas.jahnke@dlr.de

Thermochemical energy storage (TCES), where thermal energy is stored in a reversible chemical reaction in a porous powder bed, is a promising technology for large-scale and long-term thermal energy storage. It has been under long-standing investigation for prospective applications, such as the capture of excess heat from industrial processes or storing energy in concentrated solar power plants, to offset their unpredictable energy generation. This study investigates TCES in the SrBr₂-system, which offers a high energy capacity and near-perfect reversibility.

However, the scaling up of these reactors is hindered by the limited heat transfer from the heat source, such as reactor walls, to the powder bed. To address this challenge, heat conducting structures, such as fins, are incorporated into the bed to enhance thermal contact and shorten transport paths. Moreover, structural changes through mechanical and physical alteration of the powder bed, as well as changes in the microstructure, lead to changing heat and mass transport properties of the porous medium during cycling [1]. Additionally, deformation of the bed can lead to detachment from the heat conducting surfaces (see Fig. 1).

Even though physical modeling these effects can be done in principle [2], developing and parametrizing these models is challenging due to the substantial structural changes happening on multiple scales in the reacting bed. In this contribution, we attempt to overcome these challenges through hybrid modelling, i.e. the combination of physical and data-driven methods.

To this end, experimental work is carried out on the macroscale (cm) by thermochemical cycling reactive beds within reactors and measuring conversion and local temperatures inside reactors over time. In addition, imaging of the microstructure (μm) is done using μCT imaging of smaller samples, which can be used to compute effective transport parameters (see Fig. 2). Then, the available data is used to build a multi-scale model, combining data-driven techniques and physical simulations.

In a second step, ML-techniques are used to improve the heat transfer inside the reactor by designing optimized heat conducting structures. As direct simulations are prohibitively time consuming, we construct an ML-Based surrogate model, which is trained with a representative sample of physical simulations, and which can predict the performance of the reactor based on the structures' geometry. This can be done either by training a neural network on simulated data or by using techniques, such as model order reduction, where the non-linearities are handled by a neural network. The surrogate model is then coupled with a topology optimization algorithm based on the level-set method (see Fig. 3), which is used to calculate optimal geometries for the heat conducting structures. Our contribution will center on the modeling techniques employed and the preliminary optimization results obtained.

Figures attached:

Figure 1: SrBr-Powder Bed in a TCES reactor with heat conducting structures after thermochemical cycling.

Figure 2: Computation of the effective powder heat conductivity on the microscale using segmented μCT-image data.

Figure 3: Topology optimization of a reactor design with state variables: (top, left) phase function, (top, right) temperature, (bottom, left) pressure, (bottom, right) conversion.

Country:

Germany

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Student Awards:

Water & Porous Media Focused Abstracts:**References:**

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322

Beyond Biot –Nonlinear Stiffening in Fluid-Saturated Porous Media**Author:** Axel Dorian PIEPI TOKO¹**Co-author:** Ruud Weijermars ²¹ *University of Cape Town (UCT), Department of Mathematics and Applied Mathematics*² *College of Petroleum Engineering (CPG) at the king fahd university of petroleum & minerals (KFUPM)***Corresponding Authors:** pptaxe001@myuct.ac.za, ruud.weijermars@kfupm.edu.sa

This paper comprehensively investigates the elastic behavior of fluid-saturated porous media, particularly under varied stress and pore pressures. We use a Linear Superposition Method (LSM) to quantify stress distribution and effective bulk moduli within a synthetic micropore model under both drained and undrained conditions. Our results reveal a significant nonlinear stiffening effect, particularly at high pore pressures, where the bulk modulus increases with porosity—in some cases by up to 25%. This behavior deviates from predictions made by conventional poroelasticity theories relying on a priori upscaling methods. Our posteriori upscaling approach highlights the limitations of these macroscopic approaches, which often overlook critical microstructural details such as pore size distribution, pore pressure effects, and localized stresses. These findings suggest poroelasticity is better understood as a nonlinear, pore-scale phenomenon rather than an inherent material property. We therefore propose a practical method for upscaling micropore model results into an analytical expression, with direct applications in geomechanics and reservoir engineering.

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References:

324

Transformers Approach for Fracture Network Modeling: A Case Study in Kazakhstan

Authors: Timur Merembayev¹; Yerlan Amanbek²

¹ *Nazarbayev University, Almaty*

² *Nazarbayev University*

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The main goal of fault modeling is to build a network of underground faults close to reality, solving the problems of flow and transport. Simulating a fracture geometry system using the geotechnical aspects requires significant computational resources. Traditional stochastic algorithms for fracture network characterization are based solely on statistical inference from fault inputs. Hence, the resulting models may not be physically realistic as they may not be consistent with the fracture propagation and termination process.

In this presentation, we extend the fracture network model introduced in [1, 2]. The problem of recreating fault network modeling has been defined and formulated within the framework of applying a deep learning approach. We are looking at the transformer approach to recreating fracture networks for a new field based on the historical and well-known geology area. Transformers effectively capture long-range dependencies and can be adapted for sequential or spatial data. The condition transformer is useful for more context-aware network generation for external variables like stress fields or geological properties. Additionally, we used Visual Transformer to work directly with fracture network images. Transformers provide a powerful framework to generate geologically plausible fracture distributions.

This approach scales efficiently and can enhance fracture modeling by considering fractures' physical and mechanical characteristics. The application and effectiveness of this approach have been demonstrated in the geological data of the Republic of Kazakhstan.

Country:

Kazakhstan

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Student Awards:

Water & Porous Media Focused Abstracts:

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References:

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MS09 / 325

Laminar to Turbulent Convection in Porous Media: The Role of Solid-Fluid Conductivity Ratios and Porosity Variations

Author: Dario Schwendener¹

Co-authors: Xiangzhao Kong ; Jerome Noir ¹; Christophe Coreixas ²; Jonas Latt ²

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Transition from laminar to turbulent flow within the framework of conjugate heat transfer in porous media occurs in various applications across different scales, including geothermal energy extraction, thermal energy storage systems, high-temperature gas-cooled reactors, and microchip cooling. Understanding this transition is critical for optimizing systems designed to maximize surface area for efficient heat and mass transfer.

To tackle the regime transition, we developed an advanced lattice-Boltzmann Method (LBM) solver optimized for simulating conjugate heat transfer in porous media. Built on the STLBM open-source platform, the solver integrates thermo-physical heterogeneity and supports multi-threaded, parallelized computations on both CPUs and GPUs. It accurately captures the Navier-Stokes–Fourier dynamics under the Boussinesq approximation, providing a robust framework for analyzing heat and fluid flow in porous structures, including inertial effects and thermophysical heterogeneity.

Using staggered isotropic porous media composed of cylindrical structures, we investigate the effects of porosity, solid-to-fluid conductivity ratio, and Rayleigh number on overall dynamics, including Nusselt number, Reynolds number, and boundary layer thickness. In pure hydrodynamics, increasingly confined pore space strongly influences the transition from Darcy to non-Darcy flow as porosity decreases from 45% to 30%. Extending this analysis, we explore natural convection behavior during the transition from Darcy to non-Darcy (Forchheimer) flow, focusing on Darcy numbers around 10^{-6} . Our simulations further assess the impact of conductivity ratios (0.1 to 10) on convective dynamics across Rayleigh numbers spanning four orders of magnitude (10^7 – 10^{10}).

Our results reveal that inertial forces drive regime transitions from steady-state to oscillatory convection, as evidenced by spatial Reynolds number analysis. Nusselt–Rayleigh scaling in steady-state convection aligns with the classic $Nu \sim Ra$ at low porosities but deviates significantly at higher porosities. For low porosities, the transition to oscillatory convection is strongly influenced by the solid-to-fluid conductivity ratio. At high Rayleigh numbers, higher kinetic energy does not necessarily enhance heat transfer, as boundary layer thickness is influenced by both velocity and the thermal conductivity of the solid and fluid phases. Furthermore, within the examined Darcy numbers, the pore-scale Prandtl number fails to reliably predict the transition to the Forchheimer regime.

Country:

Switzerland

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Student Awards:

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MS11 / 327

Probabilistic learning of gas wall interaction from molecular Dy-

namics simulations and applications to gas transport problems in nano micropores

Author: Quy Dong To^{None}

Co-author: Christian Soize

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Modeling and characterizing gas-wall interactions at the atomic scale are crucial for understanding transport behavior in micro- and nanopores and for accurately simulating gas flows in porous materials. It is well known that gas displacement in extremely tight channels is complex and significantly influenced by adsorption/desorption physics and surface diffusion mechanisms at the boundary walls. In this work, the collisions of helium atoms with graphite plates in thermal equilibrium are simulated using Molecular Dynamics methods at various temperatures [1](#). It is observed that at temperatures as high as 200 K, gas atoms reflect almost instantaneously, and pre- and post-collision velocities are strongly correlated. However, at lower temperatures, a significant proportion of gas atoms are adsorbed and move randomly on the surface before being desorbed. The velocity correlations are also weaker and reduced with temperature. A detailed analysis of the Potential Energy Surface (PES) and Mean Square Displacement (MSD) reveals a two-stage ballistic-diffusive behavior under weak energy barriers and low friction conditions. The velocity correlation coefficient, which is directly related to the tangential momentum accommodation coefficient (TMAC), is also determined, and an empirical relation between TMAC and temperature T is proposed.

From the collision data, including particles' velocity, residence time, and surface displacement, a surrogate stochastic wall model is constructed using probabilistic learning approaches [2](#). The model is designed to replace atomic walls by predicting the probability distribution of residence time τ , surface displacements Δ_x, Δ_y , and post-collision velocities v_x, v_y, v_z for a given pre-collision velocity v'_x, v'_y, v'_z in the form:

$$(v_x, v_y, v_z, \Delta_x, \Delta_y, \tau) = f(v'_x, v'_y, v'_z, U)$$

The latent gaussian variables U are reduced unknowns representing the microstate of the solid walls at temperature T . The function f is composed of orthogonal polynomials of random variables, whose parameters are determined by minimizing probalistic distance. Since the data is generated under equilibrium conditions, special attention is given to ensuring the equilibrium distribution of classical particle velocities and respecting the principle of time reciprocity. An example of a Monte Carlo simulation of Knudsen diffusion for gas particles traveling between two parallel walls using the stochastic wall model is presented.

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Country:

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Student Awards:

Water & Porous Media Focused Abstracts:

References:

On Darcy-Forchheimer gravity currents in porous media

Authors: Sepideh Majdabadi Farahani¹; Luca Chiapponi²; Alessandro Lenci³; Sandro Longo⁴; Vittorio Di Federico¹

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Gravity-driven flows in porous media play a vital role in numerous energy and environmental applications, such as CO₂ sequestration, oil and gas reservoir management, underground hydrogen storage, geothermal energy, and pollutant transport.

We theoretically and experimentally study one-dimensional flow of gravity currents (GCs) of a Newtonian fluid advancing within an infinite, homogeneous and saturated porous domain over a horizontal impermeable bed. Both plane and axisymmetric geometries are considered. The driving force is due to the density difference between the denser flowing fluid and the lighter, immobile ambient fluid. The current is taken to be in the Darcy-Forchheimer regime, where an additional term, quadratic in the seepage velocity, accounts for inertial contributions to the resistance beyond Darcy's linear regime. The volume of fluid within the current varies as a power function of time with exponent γ ; varying values of γ parameterise the case of constant volume ($\gamma = 0$), of constant ($\gamma = 1$), waning ($\gamma < 1$), and waxing inflow rate ($\gamma > 1$).

The flow problem, governed by the interplay between viscous and buoyancy forces, is approached with the classical assumptions of the lubrication theory and of negligible thickness of the current with respect to the ambient. A nonlinear second order partial differential equation (PDE) results, which is amenable to a fully numerical solution together with associated local and integral boundary conditions. The only parameter appearing in the dimensionless PDE is a pure number N proportional to the ratio between buoyancy and viscous forces squared, i.e. a modified Grashof number; N values in practical applications vary in a large interval around unity.

A local Forchheimer number F is defined by the product of number N and the local slope of the current profile. The problem admits self-similar solutions reducing the PDE to an ODE for two limiting conditions, $F \ll 1$ and $F \gg 1$. The ODE is easily solved analytically for $\gamma = 0$, and numerically for $\gamma > 0$. The asymptotic behaviour of the self-similar solutions is in excellent agreement with the numerical results of the direct integration of the full problem. A fully analytical self-similar solution is also derived for plane geometry and $\gamma = 2$. For values of the γ parameter larger than the threshold values $\gamma = 2$ (plane geometry) and $\gamma = 3$ (axisymmetric geometry), the solutions are asymptotically invalid as the aspect ratio and the average slope of the current increase with time.

Experiments conducted for the plane case with a porous medium made of large glass beads corroborate the theory. First, the two parameters of the Darcy-Forchheimer equation were determined performing preliminary experiments. Then, sixteen experiments were conducted with three different grain sizes of the porous medium and different inflow rates ($N \in [2.8, 64]$): the experimental nose speed and current profiles are in good agreement with theoretical predictions.

Country:

Italy

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Student Awards:

Water & Porous Media Focused Abstracts:

This abstract is related to Water

References:

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- [3] Majdabadi Farahani S, Chiapponi

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329

Mineralogical and Saline Water Effects on Sandstone Reservoir in Southern Indus Basin: Unlocking EOR and CO₂ Storage Potential

Author: Bilal Shams¹

Co-authors: Darya Khan Bhutto ¹; Gul Hasnain ¹; Huzaifa Ghani ; Najeeb Anjum Soomro ¹; Rashid Mustafa Korai ¹; Suresh Kumar ; Muhammad Aleem Zahid ²; Nasrullah . ³; Osama Ajaz ⁴

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ABSTRACT

The sandstone reservoirs of the Southern Indus Basin, particularly the ones in the Pab range near Winder, Baluchistan, Pakistan, have yet to be exploited with regard to the potential for enhanced oil recovery (EOR) and carbon capture and storage (CCS). The preliminary study on mineralogical composition and the effects of saline water concentration on wettability alteration and interfacial tension (IFT) has been conducted, with implications for both on hydrocarbon recovery and on CO₂ storage.

XRD analysis shows the mineralogical profile of the sandstone, which consists of quartz at 54.67%, and other minerals, such as hematite and calcium oxide. Quartz is a key mineral that maintains structural stability and supports favorable fluid-rock interactions. The presence of hematite and calcium oxide affects the reactivity and wettability. These mineralogical characteristics are important in optimizing EOR and creating the right conditions for CO₂ storage by modifying petrophysical properties such as pore connectivity and surface wettability.

Core plugs were prepared from sandstone outcrop samples, and experimental tests were performed. Saline water flooding was analyzed through IFT measurements by pendant drop method and wettability tests by sessile drop technique across the range of saline concentrations from 1,000 to 35,000 ppm. Spontaneous imbibition tests were also conducted to find the oil recovery efficiency under various salinity levels. The results showed that increased saline concentration decreased IFT dramatically and changed the wettability from oil-wet to water-wet, improving oil displacement.

These results are consistent with international research on analogous quartz-rich reservoirs, which have been proven to be suitable for both EOR and CO₂ geologic storage. The mineral composition and salinity-induced changes in petrophysical properties are consistent with conditions that have been demonstrated to enhance the efficiency of CO₂ trapping by capillary and dissolution mechanisms.

This pioneering research fills a critical gap in understanding the interplay between mineralogy, saline water concentration and reservoir performance in the Southern Indus Basin. It offers a path forward for integrating EOR and CCS in Pakistan, utilizing local geological resources for energy sustainability and climate change mitigation.

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MS05 / 331

A comprehensive study of bacterial cells reactive transport in porous media and some applications in civil and environmental engineering.

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It is now well known that we live in a microorganism's world. Indeed, microorganisms are everywhere on earth including in unsuspected places such as the troposphere, deep frozen lakes, deep aquifers, pristine media or highly aggressive environments with extreme pH, temperatures, toxic elements concentrations... This means that they are capable of moving or being mobilised through almost all environments, and colonizing all ecosystems including the human body through symbiosis or close associations. Their ubiquity, due universal occurrence and ever increasing field application by humans and animals (field application of manure and sewage sludge, intensive farming, bioremediation,...), combined with their almost infinite metabolic potential make bacteria powerful allies in numerous human applications such as water and soil treatment, civil engineering, environmental restoration, pollutant degradation, etc. However, many applications remain limited or impossible due to our lack of understanding of the fine mechanisms by which bacteria are transported in the environment, particularly in porous media. Industrial processes based on injecting selected bacteria into soils or sediments are emerging in the context of in situ bio-reinforcement, metal bio-leaching, bio-augmentation, etc. It is therefore crucial to improve our understanding of the transport and retention of bacteria in porous media in order to predict and control their diffusion in the environment. In this context, we studied and modeled the factors controlling the mobility of several bacterial species of specific interest (*Agrobacterium tumefaciens*, *Escherichia coli*, *Cupriavidus metallidurans* CH34, *Pseudomonas putida* and *Sporosarcina pasteurii*) in porous media using a column approach. Various physical and chemical factors influencing the transport of the five bacterial species were studied in water saturated columns. The experimental and modelling results showed that these factors have a variable effect on the mobility of these model bacteria (bacterial species, cell concentration, ionic strength, solution composition...), while others have much smaller effects (cell size, pH, water flow rate, etc.). On the basis of these results, we have been able to effectively use bacterial cells injection in porous media in several types of application. For instance, we were able to bioreinforce different porous materials from river dykes in order to strengthen dykes and industrial soil environments. We were also able to apply the technology of selected bacteria injection to mobilize metals of interest from several types of materials such as polluted soils, mine tailings and waste from Electrical and Electronic Equipments (WEEE). This was done with a view to valorisation through the development of nature based solutions that can be transposed to various conditions, contexts and scales.

Keywords:

Bacterial cells, reactive transfer, porous media, columns, breakthrough curves, solution geochemistry, water flow, pH, transport modeling

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334

Complex Interactions and Flow Mechanisms of Shale Oil in Nanopores: Insights from Molecular Dynamics Simulations

Authors: Tianhao Li¹; Hai Sun¹; Zheng Li²; Dongyan Fan¹; Lei Zhang¹; Jun Yao¹

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Understanding the occurrence and flow mechanisms of shale oil in nanopores is critical for advancing knowledge of fluid behavior in porous media. Previous studies have often overlooked key factors such as the multi-component nature of shale oil, the realistic properties of nanopore walls, and nanopore flexibility, resulting in limited understanding of shale oil's behavior in nanoconfined spaces. In this study, molecular dynamics simulations were used to systematically investigate the occurrence and flow mechanisms of fluids in graphene, hydroxylated quartz, and rough kerogen nanopores. By comparing the flow of single-component and multi-component shale oil in relatively smooth quartz and rough kerogen nanopores, we found that slip flow only occurs under idealized conditions (single-component oil and smooth surfaces), whereas realistic shale oil in actual nanopores exhibits no slip flow. By studying the changes in fluid velocity profiles under different pressure gradients, we identified the critical pressure gradient for fluid flow regime transitions. Above this critical pressure gradient, the velocity profile changes from parabolic to plug-like. This phenomenon occurs because the increasing pressure gradient causes fluid near the wall to desorb and aggregate into clusters in the center of the pore. Through statistical analysis of the interaction forces between the fluid and the pore wall, we observed an increase in the vertical force exerted by the wall on the fluid, suggesting that the pressure inside the nanopores increases. To address this, we further investigated the flow of n-octane in rigid and flexible graphene nanopores. The results revealed that fluid flow in nanopores induces changes in pore pressure and pore deformation. In rigid nanopores, pore pressure increases with the rise in the pressure gradient, whereas in flexible nanopores, pore width increases with the pressure gradient. The increase in nanopore pressure or expansion of nanopores is attributed to enhanced collisions between fluid-fluid atoms and fluid-wall atoms caused by fluid flow. This study unveils the complex interactions of shale oil within nanopores, providing theoretical support for understanding the flow of shale oil in porous media and contributing to the efficient extraction of shale oil in unconventional reservoirs.

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335

Numerical Simulation of Multi-component Salts Dissolution Process Using the Lattice Boltzmann Method**Authors:** Wenxin Yang^{None}; Lei Zhang^{None}; Dongyan Fan^{None}; Jun Yao^{None}; Shuaishi Fu^{None}**Corresponding Author:** yangwenxin0223@163.com

In underground salt cavern hydrogen storage and carbon dioxide geological sequestration, water injection salt dissolution technology is widely used for artificial excavation and expansion of salt caverns. In dissolution-type geothermal energy development, this process plays a crucial role in determining reservoir permeability and hydrothermal flow behavior. During the actual water injection salt dissolution process, multiple salt phases with different properties are often involved, and significant competitive interactions exist among these phases. This competition is primarily manifested in differences in diffusion rates, dissolution rates, and ionic concentration equilibrium constraints. The dissolution of one salt phase alters the ion concentration in the solution, thereby inhibiting or promoting the dissolution of other salt phases, leading to increased complexity in interface dissolution behavior. This competitive mechanism has a profound impact on dissolution rates, interface morphology evolution, and dynamic changes in the chemical environment of the solution.

Based on the lattice Boltzmann method (LBM), this study establishes a numerical model capable of simulating the dissolution dynamics of multi-salt systems. The model incorporates the coupling mechanisms of dissolution reactions, ion diffusion, and fluid flow, while also introducing thermodynamic equilibrium conditions and chemical reaction kinetics descriptions for multi-salt systems. By simulating the dissolution behavior of different salt phases, the study systematically investigates the effects of dissolution rates, interface evolution, and ion competition on the dissolution process. Additionally, the influence of fluid flow velocity and solution concentration on the dissolution process is analyzed. The results show that the dissolution rates and interface morphology evolution of different salt phases are significantly dependent on their solubility characteristics and ion competition effects in the solution. This research provides theoretical insights into the mechanisms of multi-salt dissolution and lays an important foundation for its application in environmental science, resource development, and chemical engineering.

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References:**Plenary Lecture / 336****Land Disposal of PFAS-Contaminated Soils: A Mathematical Modeling Framework for Site-Specific Risk Assessment****Authors:** Linda Abriola¹; Uriel Garza-Rubalcava^{None}; John Christ²; Litzy Guevara¹

Co-authors: Johnathan Peck ¹; Matthew Woodcock ¹; Christopher Pisarri ³; Lesa Zimnawoda ⁴; Kurt Pennell ¹

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Per- and polyfluoroalkyl substances (PFAS), a class of some 12,000 chemicals, are recognized as contaminants of emerging concern by the US Environmental Protection Agency, which has recently promulgated stringent (part per trillion) nationwide drinking water standards for a few of the most prevalent of these compounds. Historically, PFAS were essential ingredients of aqueous film forming foams (AFFFs), and their use for fire mitigation has led to widespread PFAS contamination of soils and groundwater at airports, fire stations, and military bases across the United States.

This presentation provides an overview of recent work designed to formulate and demonstrate a mathematical modeling approach that will support the development of site-specific screening levels for PFAS-contaminated soil disposal. Mathematical modeling of PFAS transport in soils presents some unique challenges, due to the amphiphilic properties of PFAS which facilitate air-water interfacial accumulation that can affect both water flow and contaminant retention in the soil profile. The laboratory-validated multiphase flow and transport model used in this study incorporates: (a) natural recharge, (b) PFAS leaching from contaminated soils, (c) PFAS sorption/desorption in the underlying soil profile, (d) competitive PFAS accumulation at air-water interfaces, and (e) vertical advective and dispersive fluxes of constituents through the soil to the underlying groundwater.

The site selected for model demonstration is a US military base in a semi-arid region subject to long periods of cold climate conditions, necessitating the modeling of the effects of snow accumulation and snowmelt on recharge. PFAS-impacted soil, attributed to the historic use of AFFFs, was emplaced in a lined stock-pile and sampled to characterize hydrogeochemical properties and quantify contamination levels. Soil borings of the native soil within the vadose zone underlying the stock-pile were also retrieved for characterization. To quantify PFAS desorption kinetics and sorption isotherms for the PFAS-contaminated and underlying soils, a series of batch experiments was undertaken. Column experiments were also conducted to investigate PFAS leaching and subsequent transport within the underlying native soil. Data derived from these experiments were then used to parameterize the simulator for site-specific application.

Results of laboratory analyses revealed detectable concentrations of five EPA-regulated PFAS (PFOA, PFNA, PFBS, PFHxS, and PFOS) and provided information to characterize sorption/desorption and interfacial accumulation behavior. A suite of simulations was conducted for alternative site scenarios, encompassing varying contamination levels, sorption characteristics, hydraulic soil properties, and projected climatic conditions over a one-hundred-year time frame. These simulations provide site-specific estimates of projected PFAS arrival times, concentrations, and mass fluxes at the water table, as well as their ranges of uncertainty. Model-predicted PFAS fluxes are now being employed to explore the potential implications of contaminated soil leaching on groundwater quality and risk to human and ecological receptors.

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United States

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337

The high-pressure fracturing fluids invasion and its controlling factors for shale gas reservoirs using gradient nuclear magnetic resonance method

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The injection of water-based hydraulic fracturing fluids (HFF) into tight shale gas formations can significantly increase the possibility of fluids interacting with the reservoir rocks, causing damage to gas flow capacity of shale stimulated fracture network due to stress sensitivity after water invasion. As a result, it is significant to clarify the high-pressure fracturing fluids invasion within the shales, which helps to understand stress-dependent permeability alteration for the fracturing fluids-invaded shales. However, it is difficult to characterize the invasion and distribution of high-pressure fracturing fluids within shale reservoirs. In addition, the fracturing fluids invasion mechanisms for shale stimulated fracture network are not yet clear. Therefore, in this paper, by means of innovatively using low-field high pressure gradient nuclear magnetic resonance online displacement, the high-pressure fracturing fluids invasion within shale at different times and its controlling mechanisms were revealed. The results were presented as follows: it showed that only one clear single peak structure existed on the left side of NMR-T2 spectrum curves for shale matrix imbibing water, indicating that water absorption mainly occurred into shale matrix micro-nano pores during water intrusion process. The T2 spectrum surrounding area and the right-direction-shifting rate of left peak were positively correlated with matrix permeability, water injection pressure difference, and clay mineral content. It indicated that the filling of water into shale matrix would firstly occur in micro-nano pores, followed by large pores observed from NMR-T2 spectrum curves. With the increase in invasion durations, water saturation propagated in a progressive pattern of upward and downward fluctuations along the direction of water invasion within deeper matrix. It was found that the water invasion distance within shale matrix increased with invasion time, following the power function. The water imbibition distance generally could reach between 4cm~6cm within shale matrix cores of 0.000654mD~0.0068mD at high driving pressure of 15MPa~35MPa. The degree of high-pressure water invasion in shale matrix was linearly positively correlated with matrix permeability, water injection pressure difference, and clay mineral content. This paper gave insights into the high-pressure fracturing fluids invasion within shales. It provided scientific reference for reducing the stress sensitivity and alleviating reservoir permeability damage after hydraulic-fracturing process for shale gas wells.

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MS23 / 338

Molecular Mechanisms of Hydrogen Leakage and Blockage in Kaolinite Nano-Cracks for Underground Hydrogen Storage

Authors: Zheng Li¹; Tianhao Li²; Leran Meng²; Xiaoguang Wang¹; Hai Sun²; Mingshan Zhang³; Jianlong Kou⁴

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Underground H₂ storage in saline aquifers is critical for advancing the global energy transition through large-scale H₂ utilization. However, cyclic stress-induced nano-cracks in caprocks may lead to leakage due to H₂'s small size and high diffusivity. This study employed molecular dynamics simulations exploring the occurrence states of H₂ and H₂O near kaolinite surfaces, particularly focusing on H₂ leakage when a nano-crack formed. We examined the effects of basal surfaces (gibbsite and siloxane), water content, and cushion gases (CH₄ and CO₂). In gibbsite aquifers, H₂O formed adsorption layers; while in siloxane aquifers, it appeared as droplets or bridges. Upon nano-crack formation, initial H₂ leakage occurred but halted once a critical number of H₂O blocked the crack. H₂ leakage was generally higher in siloxane than in gibbsite aquifers, except at low water content. Increased water content significantly reduced H₂ leakage in gibbsite aquifers by rapidly achieving the critical H₂O number, whereas the effect in siloxane aquifers depended on H₂O distribution. Cushion gases effectively mitigated H₂ leakage. CO₂ outperformed CH₄ in gibbsite aquifers, while their effects in siloxane aquifers varied based on H₂O distribution. CH₄ reduced leakage by hindering initial H₂ entry into the crack, while CO₂ not only impeded initial H₂ entry but also assisted H₂O in blocking the crack. Our analysis of density distributions, leakage dynamics, molecular configurations, and excess chemical potentials provides insights into H₂ leakage and blockage mechanisms in aqueous environments near caprock minerals, facilitating the evaluation of H₂ storage feasibility in saline aquifers.

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Poster / 340

Exploring impacts of fungal biofilms on porous media flow

Author: ChunKi Fong¹

Co-author: Sang Hyun Lee

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Filamentous fungi play critical roles in nutrient and carbon cycling¹, bioremediation², biofouling of engineered materials³, and infection of immunocompromised individuals^{4,5}. While these processes often involve porous media flows, we have limited knowledge on fungi-fluid interactions in pore spaces. This knowledge gap restricts our capacity to control and harness fungal activity for beneficial applications. To address this, we conducted microfluidic experiments to visualize fungal mycelia and fluid flow at pore scale. *Fusarium oxysporum* was chosen as the model fungus due to its wide-spread presence and pathogenic nature in immunocompromised individuals^{4,5} and crops⁶. Single straight channel and porous media polydimethylsiloxane (PDMS) microfluidic chips designs were fabricated to analyze fungal biofilm at a single- and multi-colony levels. In addition, while straight channels can reflect microchannels in physiological or medical systems, the porous media chip could mimic soil or filter environments. Pressure sensors were incorporated to assess permeability and preferential flow paths were visually confirmed through microscope. Additionally, confocal microscopy was employed to visualize and analyze the spatial patterns and structures of fungal mycelium. We anticipate that these findings will shed light on the interaction between fluid dynamics and fungal biofilms, offering valuable insights for predicting fungal activities such as nutrient transport and bioremediation, as well as informing strategies to control fungal contamination in agricultural and medical settings.

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Country:

USA

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Poster / 343

New approach to evaluate breakthrough pressure using MICP

Authors: Rodrigo Nagata¹; Anderson Camargo Moreira²; Iara Frangiotti Mantovani²; Celso Peres Fernandes²

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Geological carbon sequestration, the capture and underground storage of CO₂, is widely considered the primary approach to offset CO₂ emissions from large-scale fossil fuel consumption. A key requirement for any potential storage site is the presence of an effective caprock. The caprock's sealing capacity, or its ability to prevent CO₂ escape, is critical in any proposed storage project [1]. One of the most important properties to evaluate the caprock's sealing capacity is the breakthrough pressure (also known as threshold pressure). It can be defined as the pressure in the nonwetting phase necessary to displace the wetting phase in a way that a continuous flow is established [2]. Due to their simplicity, quickness and low cost, Mercury Intrusion Capillary Pressure (MICP) is commonly used to measure breakthrough pressure. This method uses high pressure to force mercury (nonwetting fluid) into the sample pores. The Washburn equation relates pressure and pore size [3]. Typical MICP results are shown by plotting the accumulated volume of intrude mercury against the injection pressure. These values are converted from the mercury–air–rock system to other systems of interest, for example, the CO₂ –brine –rock system, considering the contact angle and interfacial tension. The breakthrough pressure may be determined by analyzing changes in the curvature of this curve [4], but often, this pressure is not clearly defined: the mercury appears to gradually penetrate the pore system without an evident critical pressure, indicating the abrupt formation of a percolating cluster. To overcome this difficulty, a new procedure in the mercury intrusion experiment, before the MICP curve analysis, is proposed to identify the breakthrough pressure. This method consists of the insertion of a relatively big artificial pore after a layer of the sample. This way, a pronounced intrusion is recorded when the mercury percolates the sample and reaches the artificial pore. So far, the results show that this approach is promising, with some experimental hurdles still to be overcome.

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MS17 / 344

Stochastic Analysis of Shear-Thinning Fluid Flow and Heat Transport in Geological Fractures

Author: Alessandro Lenci¹

Co-authors: Yves Méheust ²; Maria Klepikova ³; Daniel Tartakovsky ⁴; Vittorio Di Federico ⁵

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Engineered shear-thinning (ST) fluids, including polymer-based solutions, attracted considerable interest in subsurface applications for optimizing fluid circulation, transporting remedial amendments, and sweeping non-aqueous liquids in enhanced oil recovery (EOR). In this study, a stochastic analysis based on the Monte Carlo method is carried out to investigate how variations in fracture characteristics (e.g., aperture, roughness) and fluid properties (e.g., rheological parameters, polymer concentration) affect coupled flow and heat transport within a single geological fracture.

An ad hoc two-dimensional numerical model was developed to manage numerous realizations, (i) incorporating key uncertainties associated with heterogeneity and (ii) accurately representing the ST behavior of the fluid. To validate the robustness of the modeling framework, reference simulations were performed using COMSOL Multiphysics, confirming the model's ability to replicate essential flow and thermal transport phenomena. Under high-shear conditions, the ST rheology induces a spatially dependent decrease in viscosity, which influences effective transmissivity and thus heat exchange efficiency [1](#). By adjusting polymer concentration, operators can modulate the nonlinear rheological response of these fluids, tailoring their flow properties to specific geometrical and hydro-mechanical requirements.

Beyond elucidating the behavior of these fluids within a single fracture, the findings of this study are pivotal for evaluating their potential use in heat tracer tests. By varying polymer concentration, it becomes possible to generate multiple and distinct breakthrough signals in a single experiment, thereby enhancing the inference of geometrical parameters and providing more comprehensive datasets for estimating critical subsurface properties (e.g., fracture aperture, aperture fluctuations, and thermal conductivity). Overall, the proposed Monte Carlo framework offers new insights into the interplay between nonlinear rheology and fracture geometry, ultimately supporting advanced subsurface characterization and more effective tracer-based investigations.

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Poster / 345

Molecular dynamics insights into hydrogen storage in porous media

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Hydrogen geologic storage offers significant potential to enhance energy sustainability, but optimizing its storage remains a challenge. Key to addressing this challenge is understanding the thermodynamic processes within mineral nanopores in underground formations. These nanopores present unique opportunities and challenges due to their complex surface chemistry and interactions with surrounding particles under variable stress conditions. This study uses molecular dynamics (MD) simulations to investigate how hydrogen interacts with porous rock matrices at the molecular level, with a particular focus on energy changes and the role of local stresses in hydrogen storage and recovery.

The primary objective of this research is to examine the interaction dynamics between hydrogen molecules and surrounding particles in geological nanopores, with a focus on how local matrix properties and applied stress affect storage efficiency. We employ MD simulations to model hydrogen adsorption and reaction processes under conditions typical of underground environments. The study particularly emphasizes how hydrogen density, adsorption capacity, and reaction pathways are influenced by the surface chemistry and stress conditions of the mineral matrix.

Our simulations reveal key insights into hydrogen adsorption and reaction dynamics within nanopores. Pyrite (FeS₂), a mineral associated with hydrogen sulfide (H₂S) production, demonstrated lower hydrogen adsorption capacities compared to other minerals like calcite and quartz. The weaker interactions between hydrogen and the pyrite surface resulted in less efficient adsorption. In the presence of elevated temperatures and water, reactive MD simulations showed that H₂ dissociates into H⁺ and S²⁻ ions on pyrite, promoting H₂S formation. Beyond adsorption, we also investigate how local stresses and matrix properties influence hydrogen storage and recovery. Our simulations show that mechanical deformation or applied pressure significantly alters adsorption behavior, hydrogen density, and recovery efficiency within water saturated nanopores. Free energy calculations are used to evaluate the thermodynamic favorability of hydrogen adsorption and desorption, providing deeper insight into the feasibility of both storing and recovering hydrogen in these geological systems.

Our study provides valuable insights into improving geologic storage methods and managing sulfur byproducts like hydrogen sulfide, a key challenge in large-scale storage. Ultimately, this research contributes to the development of more efficient and sustainable hydrogen storage technologies, which are essential for advancing clean energy solutions and supporting global energy sustainability goals.

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MS07 / 346

Rigorous Upscaling of the Navier-Stokes Equations in Heterogeneous Porous Media

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Fluid flow through heterogeneous porous media is ubiquitous in a variety of subsurface engineering applications, including hydrology, geothermal energy production, hydrogen storage, and carbon dioxide sequestration. To efficiently study macroscopic fluid flow—as well as other macroscopic phenomena—in these systems, rigorous upscaling techniques can be employed to derive coarse-grained models with *a priori* error estimates and *applicability conditions* (i.e., physical conditions under which a model will meet its *a priori* error estimates). No fitting parameters are required in the formulation of such models, as the coarse-grained descriptions are derived using fine-scale information (e.g., the microstructure geometry and equations describing the fine-scale physics) to accurately account for multiscale behaviors. Despite their benefits in accuracy and efficiency, a majority of upscaling techniques depend on a strict set of methodological assumptions (e.g., diffusion- or viscous-dominated physics, periodic geometries at finer scales, scale separation, and negligible effects from the boundaries of a system) that hinder their ability to be rigorously applied in practice. To overcome these limitations, we previously developed a novel upscaling methodology, the Method of Finite Averages (MoFA), that avoids the aforementioned assumptions and provides a unique combination of *rigor* and *generality* while modeling physical phenomena in heterogeneous porous media. In this work, we apply MoFA to rigorously upscale the Navier-Stokes equations and develop a model for fluid flow in heterogeneous porous media. The resulting upscaled model rigorously accommodates temporally-varying, system-scale boundary conditions and low-Reynolds-number flows (i.e., $Re \sim 1$). We demonstrate these capabilities and discuss the computational efficiency achieved with the MoFA model through numerical validation experiments.

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MS01 / 348

The effect of random and correlated heterogeneity on CO₂ storage in saline aquifers

Authors: Ravid Rosenzweig¹; Prince Kumar²; Evyatar Cohen²; Ran Calvo²; Ran Holtzman³

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² Geological Survey of Israel

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Numerical simulations are essential for understanding the migration and trapping of injected CO₂ in saline aquifers. They allow to predict plume spreading, CO₂ dissolution, leakage rates and assess possible risks and pitfalls in the process. However, their predictive capability depends on detailed and accurate knowledge of subsurface properties, and in particular the type and degree of heterogeneity, which is often incomplete. Here, we investigate the effect of spatial heterogeneity on the migration and trapping of CO₂ in geologic carbon storage. We perform 2-D numerical simulations

of CO₂ injection and consequent spreading into aquifers having uncorrelated (random) and spatially-correlated heterogeneous permeability fields of different correlation lengths, using parameters from a potential storage site, the Negev Jurassic aquifer (Israel). We analyze the plume shape, leakage rates and the degree of trapping in the different scenarios.

We find that the type of heterogeneity significantly affects the dynamics of the CO₂ plume spreading: in the homogeneous and uncorrelated cases, the CO₂ plume rises rapidly and then spreads horizontally as a thin plume beneath the caprock. In the correlated cases, however, the plume remains in the bottom of the aquifer (further down from the caprock), where the plume primarily migrates horizontally, exhibiting a larger lateral spreading with increasing correlation length. Yet, the horizontal extent of the plume in the correlated cases remains smaller than in the homogeneous and uncorrelated cases. Consequently, in the correlated cases, CO₂ does not reach the caprock throughout the duration of the simulation, while in the homogeneous and uncorrelated cases, a negligible fraction of the CO₂ penetrates into the caprock in the form of dissolved CO₂. Heterogeneity, regardless of spatial correlation, increases the fraction of trapped CO₂ (dissolved CO₂ and capillary-trapped CO₂), and therefore the storage security.

In conclusion, we show that correlated heterogeneity substantially increases storage security and decreases risk of leakage, by keeping the CO₂ plume away from the caprock and increasing CO₂ trapping. Our study highlights the importance of detailed characterization of heterogeneity structure in sites that are considered for CO₂ storage.

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References:

MS11 / 351

Inertia effects on mixing and reactive transport in porous and fractured media

Author: Peter Kang¹

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Mixing and reaction in porous and fractured media govern a wide range of natural and engineering processes, including carbon mineralization, cave formation, geothermal energy production, contaminant transport, and microfluidics. Subsurface systems often feature fractures and conduits that serve as highways for fluid flow. Typical flow velocities in these systems are high enough to induce inertial flows, resulting in complex flow topologies. However, due to the common perception that porous media and microchannel flows are slow, the effects of fluid inertia are often overlooked in studies of mixing and reaction. In this talk, I will present our recent findings, derived from microfluidics experiments and numerical simulations, that reveal how fluid inertia fundamentally transforms reactive transport processes, including mixing-induced chemical reactions as well as mineral dissolution and precipitation. Lastly, I will illustrate how these insights can inspire solutions to critical challenges such as carbon mineralization and fracture sealing.

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352

The evolving interface in the porespace during oxidation of hydrogen on iron oxide and iron sulfide minerals at subsurface storage conditions –new insights from flow experiments

Author: Christian Ostertag-Henning¹

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Due to the demand for large subsurface storage volumes for hydrogen produced by renewable energy, different porous reservoir rocks and the related cap rocks are being investigated in Germany. The geochemical redox reactions involving either the reduction of iron in iron(III)oxides (hematite) or the reduction of sulfur in FeS(-I) sulfides (pyrite) is a not well quantified risk, even if regarded as much slower than possible microbial oxidation reactions. Therefore, different experimental avenues have been taken in the past years to understand the reactions, and quantify the rates of individual reactions and determine possible limiting factors. Up to now experiments predominantly have been carried out in static batch type reactors (e.g. Thüns et al 2019, Truche et al 2010) on sieved mineral grains with diameters near 100 µm. In these systems the evolving boundary layer on the grains – or the reaction front –may significantly retard the overall reaction progress, as the transport of the reduced products, i.e. ferrous iron or sulfide, away from the reaction front is strongly inhibited by absence of mixing or turbulence.

Therefore we developed a set of flow-through experiments aiming to investigate the magnitude of suppression of the apparent rates of hydrogen oxidation/iron or sulfur reduction. One avenues was to investigate the rates of hydrogen oxidation and iron (and sulfide) release near in situ temperatures and pressures in high-pressure gold-coated flow cells. The other avenue being developed is using microfluidic systems to be able to follow not only the oxidation of hydrogen and release of reduced products, but also to possibly delineate if these products might reprecipitate in the downstream part in chemical or physical gradients in the inhomogeneous flow system. For this, the reactions between hydrogen and the evolving pyrite/pyrrhotite or hematite/magnetite surfaces were monitored by in situ microscopy and operando Raman spectroscopy in a dedicated microfluidic system. In contrast to the processes in batch type reactors dominated by direct dissolution-reprecipitation processes for e.g. the evolving hematite-magnetite surface (cf. Ostertag-Henning & Plümper, 2024), the sites of redox reaction and dissolution in flow systems frequently are upstream of the site of secondary precipitation, increasing the risk of reducing pore throat diameters and flow conditions if the extent of the reactions is significant.

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MS08 / 353

Impact of heterogeneity and its alteration by erosion on solute transport in unsaturated media**Authors:** Ali Saeibehrouzi¹; Soroush Abolfathi²; Petr Denissenko²; Ran Holtzman³¹ *University of Warwick & Coventry University*² *University of Warwick*³ *Coventry University***Corresponding Authors:** p.denissenko@warwick.ac.uk, ali.saeibehrouzi@warwick.ac.uk, rholtzman4@gmail.com, soroush.abolfathi@warwick.ac.uk

Solute transport in unsaturated media exhibits a complex, nonmonotonic dependence on fluid saturation and flow rates. Adding to the intricate dependence of multiphase flow and solute transport on the heterogeneity across scales is their coupling: the sensitivity of the concentration fields to the spatial distribution of the fluid phases and their velocity fields.

Here, we study solute transport following partial displacement of one fluid by the other, where the fluids are immiscible and hence solute transport occurs only in one fluid and the fluid-fluid interface acts as barrier for transport.

We combine pore-scale simulations (using openfoam) with microfluidic experiments to examine the role of the pore-scale heterogeneity structure (in terms of its spatial correlation) and its evolution with chemical and mechanical erosion.

We find that increasing the correlation length in particle size increases fluid connectivity, and thus the solute spreading by reducing the number of advection-dominated regions. Decreasing saturation of carrier fluid (in which dissolved solutes are transported) is found to promote dead-ends (slow flow regions), and thus of diffusion.

We compare two simple forms of erosion in granular media: mechanical where the smallest particles are washed away, vs. chemical where all particles are shrunk by uniform dissolution. We find that mechanical erosion, unlike chemical erosion, alters the pore space morphology toward a multi-modal variation in pore sizes, which shifts transport towards a more non-Fickian spreading. For saturated media, erosion induces a non-monotonic effect on solute spreading, promoting spreading at the diffusion-dominated (low Peclet) regime while suppressing it at higher rates (high Peclet). Under unsaturated conditions, erosion decreases spreading by reducing local velocities through widening available pathways, and enhances mixing by minimizing dead-ends which enhances the relative strength of advection.

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Poster / 355

Numerical Solvers for Stationary Diffusion Problems in Digital Rock Physics

Author: Mirko Siegert¹

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Digital rock physics provides a powerful framework for characterizing the physical properties of rock samples using computational methods. In this work, we present a set of numerically efficient solvers developed for stationary diffusion problems, enabling the computation of thermal conductivity, electrical conductivity, and permittivity from micro-CT images of rock samples.

The solvers are implemented in Fortran, are freely accessible, and designed for high-performance computing across multiple CPUs without external dependencies. This approach ensures reproducibility and scalability for a wide range of applications in digital rock physics. By leveraging detailed microstructural information from high-resolution micro-CT images, our method provides the possibility to predict transport phenomena, contributing to advancements in the understanding of rock behaviour under various physical conditions.

We will discuss the numerical implementation, performance benchmarks, and validation against experimental data. The proposed framework offers a robust, open-source solution for researchers and practitioners in geosciences.

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MS24 / 356

Molecular Modeling of Structure, Diffusion, and Electrical Conductivity of Ionic Aqueous Solutions in Bulk and Confined within Nanoporous Media.

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Co-authors: Carlos Torres-Verdin¹; Julio C. Villarroel Salvatierra¹; Domenico Maria Crisafulli¹

¹ The University of Texas at Austin

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This study is part of an extensive research program focused on the use of computational simulations to analyze the diffusion and electrical conductivity of ionic aqueous solutions in bulk and under nanoconfinement. We employed molecular dynamics (MD) simulations at OPLS-AA (Optimized

Potentials for Liquid Simulations All Atom) + SPC/E (Extended Simple Point Charge) level to explore the structural and dynamic properties of sodium chloride (NaCl), potassium chloride (KCl), and lithium chloride (LiCl) in bulk aqueous solution. To quantify the effects of ion concentration and temperature, we calculated radial distribution functions (RDFs), coordination numbers, diffusion coefficients (D), and electrical conductivity for various concentrations (0.1, 0.5, 1.0, 2.0, 3.0, 4.0, and 5.0 M) and temperatures (20°C, 50°C, and 100°C). The radial distribution functions revealed that Li⁺ exhibits the lowest coordination number (3.6), indicating a compact and structured hydration shell due to its small size and high charge density. In contrast, Na⁺ (5.4) and K⁺ (6.6) show higher coordination numbers, suggesting more extended and diffuse hydration shells. These trends highlight that larger ions form less structured hydration shells with weaker ion-water interactions. It is worth noting that the coordination numbers obtained are in agreement with the experimental values reported in the literature. The analysis of diffusion coefficients reveals that heavier ions, such as K⁺ and Na⁺, under the same concentration and temperature conditions, exhibit faster diffusion within the fluid compared to Li⁺. Furthermore, as ion concentration increases, ion mobility decreases, while higher temperatures result in larger diffusion coefficients. To validate our MD model, we compared the calculated electrical conductivity values via the Nernst-Einstein equation with experimental measurements obtained using the open-ended coaxial reflection method. The results indicate that the MD simulations accurately reproduce the electrical conductivity of NaCl, KCl, and LiCl in aqueous solution at the ion concentrations studied in this work. To quantify the effect of nanoconfinement, we analyzed the structural and mobility properties of NaCl in solution confined within silica nanopores at various ion concentrations and pore sizes. The results show charge accumulation (double layer) near the surfaces of the solids. In addition, electrical conductivity increases as pore size increases. Finally, the presence of an external electric field results in increased ionic mobility and, consequently, higher electrical conductivity. These results highlight the use of MD simulations to provide a detailed molecular description of the structural properties and electrical mobility of ionic aqueous solutions in bulk and under nanoconfinement.

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Poster / 358

Operando visualization of thermogenic fluid and fracture development in shale

Author: Wen Song¹

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Ultra-low permeability shales provide a promising repository for wastes generated from nuclear energy production. Cooling of high-energy wastes, however, thermolyzes embedded organic matter into fluid phases that may lead to local stress concentration and fracturing. Understanding and controlling the fundamental THMC coupling in these heterogeneous nanoconfined environments is therefore critical to designing safe and secure nuclear waste repositories, yet much remains unresolved due to missing micro/nanoscale probes. In this talk, I will show an *operando* scanning electron microscopy (SEM) platform that enables the first *in situ* observation of coupled THMC interactions

in organics-laden shale, with ~ 2.5 nm/pixel, 10 Hz, and elemental resolutions, to constrain the necessary conditions for thermogenic pore and fracture development during high-level nuclear waste disposal. Notably, surface wetting characteristics are measured and heating-rates are mapped to constrain the conditions that enable self-sealing fluid-fracture development.

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MS06-A / 359

DNS of gas-liquid multiphase flow through FIB-SEM obtained cement-based microstructure

Author: Luka Malenica¹

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Concrete is the world's most widely used building material, and its durability has an enormous environmental and economic impact. Cement-based structures are generally under unsaturated conditions, and among the different factors, moisture conditions are directly related to many durability issues, such as freeze-thaw or corrosion-induced damages [1, 2]. Nevertheless, traditional approaches for assessing moisture state and unsaturated transport characteristics typically rely on macroscale models that utilize macroscopic properties and simplified equations, including Lucas-Washburn and Richards' equations [3]. However, observations of the actual concrete structures often do not follow behavior predicted by the mentioned conventional models, meaning that more appropriate transport models are needed. Therefore, there is a need for a better fundamental understanding of essential processes at the pore level [4]. Despite considerable advancements in recent decades, current imaging techniques still fall short in achieving the spatial and temporal resolutions required to capture the intricate dynamics of water transport in complex, heterogeneous cement-based porous media.

This work uses an actual cement-based microstructure (imaged by FIB-SEM nanotomography [5]) as a computational domain. Extensive and computationally intensive 3D direct numerical simulations (DNS)[6] of air-water multiphase flow are carried out to obtain deeper insight and consistent explanations of different processes during a water absorption event. This work focuses on providing a detailed pore-scale insight into the full interface-resolved complexity of waterfront advancement (spatially and temporally), gaining a deeper understanding of an air-trapping mechanism, and exploring the complexities of pressure distribution of residual (non-wetting) gas phase. Obtained results and conclusions improve our fundamental understanding and could significantly impact the development of enhanced macroscale models needed for practical large-scale modeling.

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MS03 / 360

Developing a Foundation Model for Predicting Material Failure

Author: Hari Viswanathan¹

Co-authors: Agense Marcato ¹; Aleksandra Pachalieva ¹; Daniel O'Malley ¹; Esteban Rougier ¹; Javier E. Santos ²; Kai Gao ¹; Ryley Hill ¹; Xiaoyu Wang ¹

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Understanding material failure is critical for designing stronger and lighter structures by identifying weaknesses that could be mitigated, predicting the integrity of engineered systems under stress to prevent unexpected breakdowns, and evaluating fractured subsurface reservoirs to ensure the long-term stability of the reservoir walls, fluid containment, and surrounding geological formations. Existing full-physics numerical simulation techniques involve trade-offs between speed, accuracy, and the ability to handle complex features like varying boundary conditions, grid types, resolution, and physical models. While each of these aspects is important, relying on a single method is often insufficient, and performing a comprehensive suite of simulations to capture variability and uncertainty is impractical due to computational constraints. We present the first foundation model specifically designed for predicting material failure, leveraging large-scale datasets and a high parameter count (up to 3B) to significantly improve the accuracy of failure predictions. In addition, a large language model provides rich context embeddings, enabling our model to make predictions across a diverse range of conditions. Unlike traditional machine learning models, which are often tailored to specific systems or limited to narrow simulation conditions, our foundation model is designed to generalize across different materials and simulators. This flexibility enables the model to handle a range of material properties and conditions, providing accurate predictions without the need for retraining or adjustments for each specific case. Our model is capable of accommodating diverse input formats, such as images and varying simulation conditions, and producing a range of outputs, from simulation results to effective properties. It supports both Cartesian and unstructured grids, with design choices that allow for seamless updates and extensions as new data and requirements emerge. Our results show that increasing the scale of the model leads to significant performance gains (loss scales as $N^{-1.6}$, compared to language models which often scale as $N^{-0.5}$). This model represents a key stepping stone to advancing predictive capabilities of material science and related fields.

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MS03 / 361

Effects of fluid inertia and variable-density flows on mineral dissolution: 3D Pore-scale simulations and millifluidics experiments

Authors: Hongfan Cao^{None}; Woonghee Lee¹; Michael Chen²; Piotr Szymczak³; Rhokyun Kwak^{None}; Peter Kang⁴

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Mineral dissolution during groundwater flow is a crucial phenomenon that has received continued interest for decades as a main drive of various subsurface processes, such as carbon mineralization, karstification, and the formation of complex rock patterns in caves. In fractured media and dissolving porous media, fluid inertia can play an important role in shaping fluid flow and dissolution processes.

For example, recent studies have reported that pore-scale vortical flows can readily occur, leading to mixing and reaction hotspots. Furthermore, as dissolution proceeds, the density of the fluid near solid fluid interfaces will increase and may lead to the density-driven convective flow. However, the effects of fluid inertia and density driven flows on mineral dissolution in fractured media have rarely been studied.

This study investigates the impact of fluid inertia and variable density flows on mineral dissolution in fractured media by combining visual laboratory experiments and three-dimensional (3D) pore-scale numerical simulations. A series of millifluidics experiments were conducted on a model single fracture/pore to examine how dissolution proceeds in the presence of inertial and density-driven convective flows. Gypsum cast from Plaster of Paris was utilized as the dissolving material in a polycarbonate flow channel. The flow channel was placed in a few different configurations, aligning the main channel flow with, perpendicular to, or against gravity, to examine the influence of changing the direction of density-driven flow with respect to the induced flow. Experiments are conducted at varying flow rates to investigate the effects of fluid inertia. To better understand the underlying mechanisms leading to different dissolution patterns, three-dimensional (3D) pore-scale numerical simulations with the same geometry used in the millifluidic experiments are performed. A micro-continuum formulation is used to numerically simulate pore-scale flow and reactive transport involving gypsum dissolution. Both the laboratory experiments and pore-scale numerical simulations indicate that the fluid inertia and density contrast resulting from dissolution can have major impacts on dissolution patterns and rates.

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MS07 / 363

Topologically-reduced models of flows in porous media with inclusions

Author: Beatrice Riviere^{None}

Co-author: Rami Masri¹

¹ *Brown University*

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Mixed-dimensional coupled problems are characterized by coupled partial differential equations defined over domains of different dimensions. Examples include porous media with embedded inclusions. These problems arise in several applications ranging from geosciences to biomedicine. These models are computationally efficient thanks to the dimension reduction of the physical problem valid in the inclusions.

This talk presents recent advances for the numerical analysis of mixed-dimensional PDEs with co-dimension equal to two. First, the convergence of a discontinuous Galerkin scheme is obtained via the derivation of a priori error bounds. The analysis is non-standard because of the low regularity of the weak solution. Second, using topological model reduction, we obtain reduced models of solute

transport in tubular-like inclusions of varying cross-section and with arbitrary axial velocity profile. Finally, numerical examples of flow in an organ and its vasculature are shown.

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MS09 / 364

A Multiscale Approach to Pore-Network Two-Phase Flow Simulation Applied to a Carbonate Reservoir

Author: Rafael Arenhart¹

Co-authors: Fernando Bordignon¹; Giovanni Formighieri¹; Leandro Figueiredo¹; Rafael Melo²; Robim Pacheco¹; Rodrigo Surmas²; Romulo Cenci¹

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Pore Network Models (PNM) are an important approach to flow simulation in porous media, alongside direct numerical simulation and Lattice Boltzmann Models. Those methods are usually applied in the context of digital rocks, in which images of rock samples are used to extract the geometric information used in the simulation. When compared to the other approaches, PNM is considered to be a more computationally efficient solution, both in processing time and memory requirements, specially for sensitivity tests where the network is extracted once and multiple simulations with diverse flow parameters are performed.

A prevalent challenge in porous media flow simulation is the handling of multiscale media: samples with a broad distribution of pore sizes. Pore sizes can be separated in two different classes of image elements, depending on the imaging resolution: resolved elements (clear distinction between void and solid space) and subresolution elements (resolved image elements containing both void and solid space). Important reservoir rock types such as carbonates present such multiscale behaviour. Multiscale models aim to address the lack of pore geometry information on the subscale phase and the computational challenge of taking in account all subscale pores in a representative volume.

There are multiple ways to include multiscale elements in PNM, such as the one proposed by Bultrays (2016), in which the extraction of the network creates two categories of pores: Navier-Stokes pores from resolved elements and Darcy pores from subresolution elements. Navier-Stokes pores are evaluated using the method by Valvatne(2004) in which a regular cross section geometry is assigned to pores and throats based on their shape factor. The present work changes the approach to the solution of the Darcy pores, using a bundle of tubes model to calculate their flow properties. This approach was selected because the bundle of tubes model may be solved with the pore radii information, which can be obtained experimentally from the readily available mercury injection capillary porosimetry (MICP) test.

The method was implemented in Geoslicer, an open source software platform for Digital Rock visualization, analysis and simulation. Simulation was performed on a pre-salt carbonate rock formation of the Campos basin and both absolute permeability and relative permeability data were obtained and compared with experimental values. Absolute permeability has shown good agreeability between simulated and experimental values. Relative permeability results showed the necessity of

parameter calibration to take into account the shape factor of subscale pores, compensate for the intrinsic subestimation of pore radius in MICP, and the distribution of contact angles. It should be noted that contact angle distribution is a complicating phenomena also present in single scale simulations.

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MS08 / 366

A Theory of Hydrodynamic Dispersion and Reaction in Porous Media Beyond the Long-Time Limit

Author: Md Abdul Hamid¹

Co-author: Kyle Smith¹

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In the literature, a range of theoretical approaches has been utilized to study solute transport through porous media. Among these, volume-averaging techniques developed by Whitaker and coworkers, alongside probabilistic methods introduced by Brenner and coworkers, have become prominent within the research community. While these approaches have proven useful, they encounter significant challenges when applied to rapidly changing transient conditions that extend beyond pseudo-steady or quasi-steady states. This study presents a novel theoretical framework for investigating transient solute transport in saturated porous media, accounting for the simultaneous effects of advection, diffusion, and reaction. In many geological, biological, and engineering systems the transient evolution of Darcy-scale concentration field is governed by complex interplay between these pore-scale processes (i.e. advection, diffusion and reaction). Due to the presence of different length scales, such systems are often analyzed using upscaled models derived through homogenization techniques. In such models, the evolution of the local volume-averaged concentration is described by a Darcy-scale mass conservation equation, which relies on upscaled transport coefficients, commonly referred to as Darcy-scale phenomenological coefficients.

The introduced transient theory is proposed for modeling solute transport through porous media comprising of both active and inactive solid/liquid interfaces. The transient problem is studied in the frequency domain by taking the continuous time Fourier transform of time dependent parameters. The mathematical formulation of the transport problem studied is presented for a repetitive unit cell that represents the porous medium. A Darcy-scale mass conservation equation is derived, incorporating three upscaled transport coefficients calculated from the periodic unit cell representation of the system. These upscaled transport coefficients are also interpreted as transfer functions defining an output-input correlations between frequency domain parameters. The first transfer function is the effective diffusion coefficient tensor, which relates the average diffusive flux (as output) to the macroscopic concentration gradient (as input). The second, the advection suppression vector, connects the fractional deviation of the advection rate from its expected value (e.g., the product of average velocity and average concentration) as the output to the pore-scale concentration difference as the input. The third transfer function, the effective reaction rate transfer function, links the average surface flux (output) to the microscopic concentration difference (input). Analytical expressions for the longitudinal component of the effective diffusion coefficient tensor in the flow direction for

Poiseuille flow through active and inactive parallel plates and circular tubes are also derived. Additionally, the theory is applied to obtain time-domain breakthrough curves for Poiseuille flow through parallel plates. The results are compared with direct pore-scale solutions and conventional theory of pseudo-steady dispersion. This comparison reveals that the proposed transient theory delivers more accurate predictions for the transient evolution of the average concentration over time compared to the conventional theory.

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MS06-A / 369

Fluid Distributions for Drainage in Open Rough-walled Fractures with Smoothly Varying Aperture

Author: Rahul Krishna¹

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Displacement of a wetting by a non-wetting fluid in fractured media is a process with relevance for many applications, such as fluid storage in the subsurface or oil and gas exploitation. Numerical modeling of flow processes in fractured media is challenging due to the very small length scales needed to resolve fracture geometries of large fracture networks. It is highly questionable if the two-phase flow equations can be simplified to continuum approaches, such as established for porous media, which would allow for coarse spatial resolutions of a model. For this reason, it is necessary to develop a good understanding of how flow conditions (in particular, the capillary number and viscosity contrast) and fracture geometry control the two-phase flow regimes, and in particular the spatial distributions of the two fluids during the displacement process. These patterns play a key role in determining the macroscopic behavior. One key properties of the flow patterns are, for example, the amount and spatial distribution of wetting fluid that is immobilized behind the displacement front. While there has been extensive investigation of this question in the context of porous media, studies on rough fractures are relatively scarce.

It is well established that in horizontal settings, the displacement is governed by capillary and viscous forces, resulting in the emergence of various displacement patterns (compact, viscous fingering or capillary fingering, and various intermediate regimes between them). For porous media flow in uniform packings and flow between parallel plates, these patterns are well quantified. If the fracture is, however, rough, i.e., with rough walls resulting in a spatially-varying aperture field, patterns can be controlled by both the structure and the flow conditions. It is not well understood, under which conditions patterns are controlled by the flow conditions or by the geometrical properties of the aperture field.

In this contribution, we perform Direct Numerical Simulation (DNS) to analyze the drainage process by solving the Navier–Stokes equations within the fracture’s space, employing the Volume of Fluid

(VOF) method to track the evolution of fluid-fluid interfaces. We consider a wide range of Capillary numbers (10^{-5} – 10^{-2}), as well as three distinct viscosity ratios (0.8, 0.05 and 0.01), and address realistic synthetic fracture geometries characterized by their Hurst exponent, the ratio of the roughness amplitude to the mean aperture, and the correlation scale of the investigated fracture domain.

We evaluate the displacement patterns based on morphological properties, such as Euler number, cluster size distribution or interfacial length, as well as on macroscopic (averaged) properties, such as volumetric fluid content. The focus is on the question, for which conditions the fracture behaves macroscopically 'smooth', meaning that the features are dominated by the flow conditions, and for which conditions the geometry of the aperture field influences these properties. As an example, we look for the geometric conditions that maximize trapping of the displaced fluid.

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MS20 / 370

Can asymmetric pores rectify fluid flow in the brain?

Author: Douglas Kelley¹

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Water-like fluids move around and through brain tissue, sweeping away metabolic wastes whose accumulation correlates with diseases like Alzheimer's and Parkinson's. Flow is driven, at least in part, by the dilation and constriction of arteries that lie within annular perivascular spaces filled with water-like cerebrospinal fluid. Naively, we would expect the oscillatory motion of artery walls to drive oscillatory flows, pushing cerebrospinal fluid out of the perivascular space when the artery dilates and drawing it back in when the artery constricts. In vivo experiments reveal just such an oscillatory flow – but accompanied by a fast, directed motion in the same direction as blood flow, deeper into brain tissue. The mechanism driving that directional flow remains unknown. In other bodily fluid transport systems, directional flow is ensured by valves, as in the heart, lymph vessels, and veins. Several researchers have speculated that artery-driven pulsation could be rectified by valve-like structures. More specifically, it may be that the narrow gaps between the astrocyte endfeet, through which fluid probably passes as it transits from perivascular spaces into the surrounding tissue, have asymmetric structures and rectify flow.

We have explored that possibility through simulations and experiments. Experiments and corresponding theory confirm that a conical pore in an elastic membrane favors one flow direction over the other. Simulations confirm that a wedge-shaped gap likewise rectifies flow, that realistic sizes and stiffnesses might produce the flows observed in vivo, and that such a valve would likely work well for frequencies associated with respiration, heart beats, and rerouting of blood (functional hyperemia), but not for frequencies associated with ultrasound. Rectification is most efficient when endfeet are neither too thick, nor too thin. Simulations also show that wedge-shaped gaps are not

the only possible valves. Overlapping endfeet of unequal lengths can rectify flow, as can the convex shape of the endfoot wall. The three mechanisms are not mutually exclusive. I will close with brief comments about open problems in brain fluid flow related to pores and poroelasticity.

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References:**Poster / 371**

Advancing Reactive Transport Simulations: The Impact of Advective/Diffusive Mineral Accessibility in Sandstones

Authors: Mohammad Kariminasab¹; Lauren Beckingham¹

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Reactive transport simulations play a crucial role in advancing our understanding of geochemical subsurface processes, such as modeling geological carbon sequestration and hydrogen storage. These simulations typically employ mass conservation equations to represent chemical reactions and transport phenomena in porous media, which can occur through dispersive/diffusive or advective mechanisms. The accuracy of these simulations depends on our understanding of fundamental formation properties, including mineral abundance, pore structure, porosity, and accessible surface area (ASA). As reactive fluids flow through interconnected pores, they interact with accessible mineral surfaces either advectively (via macropores) or diffusively (through nanopores in the clay pore network). These interactions are referred to here as advective and diffusive accessibility. Variations in accessibility can result in different reaction rates on mineral surfaces. To incorporate these variations into the model, the dispersion-diffusion tensor (D) is modified by adjusting the tortuosity (τ). The main outcomes of this study include quantifying the advective and diffusive accessibility for each mineral phase and developing a correction factor for dispersion-diffusion tensor based on clay type and thickness. These corrections are intended to improve the predictive capabilities of reactive transport models in geological studies. Using Scanning Electron Microscopy Backscattered Electron (SEM-BSE) images, processed mineral maps, and connectivity maps from previous research, diffusive and advective accessibility is determined by counting accessible mineral pixels adjacent to connected nanopores or macropores. The tortuosity value is then adjusted based on the quantified advective and diffusive accessibility for each mineral phase, along with measured clay coating thickness and clay type. Finally, simulations are compared to evaluate the impact of these modifications.

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MS06-A / 372

Accelerating multiphase simulations with denoising diffusion model driven initializations**Author:** Javier E. Santos¹**Co-authors:** Jaehong Chung²; Agnese Marcato³; Hari Viswanathan⁴; YenTing Lin⁴¹ *Los Alamos*² *Stanford*³ *Politecnico di Torino*⁴ *Los Alamos National Laboratory***Corresponding Authors:** jaehongchung@stanford.edu, yentingl@lanl.gov, agnese.marcato@polito.it, viswana@lanl.gov, javierestradasantos@gmail.com

Pore-scale simulations are computationally expensive and the presence of non-unique solutions can require multiple simulations within a single geometry. To overcome the computational cost hurdle, we propose a method that couples generative diffusion models and physics-based simulations. While training the data-driven model, we simultaneously generate initial conditions and perform physics-based simulations using these. This integrated approach enables us to receive real-time feedback on a single compute node equipped with both CPUs and GPUs. By efficiently managing these processes within a single compute node, we can continuously monitor performance and halt training once the model meets the specified criteria. To test our model, we generate realizations in a real Berea sandstone fracture which shows that our technique is up to 4.4 times faster than commonly used flow simulation initializations.

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MS22 / 373

Hierarchical Numerical Modeling of Tortuosity Modifications in Laser-Engineered Carbon-based Supercapacitor Electrodes**Authors:** Nadia Bali¹; Michail Athanasiou¹; Spyros N. Yannopoulos¹**Co-authors:** Nikolaos Samartzis¹; Athinais Mavrikaki¹; Athanasios Souliotis¹

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Fast and efficient charging in electrochemical energy storage devices relies heavily on the design of highly porous nanocarbon-based electrodes. Their hierarchical pore structure should facilitate rapid ion transport while maximizing the accessible surface area for charge storage. The microporous structure of supercapacitor electrodes plays a crucial role in their performance, affecting electronic and ionic transport properties, as well as mechanical stability, due to the non-uniform distribution of phases. Optimizing the microporous structure is essential for enabling high-rate charging, while maintaining high energy density, which is key for developing next-generation electrodes capable of overcoming transport limitations [1]. A strategy based on laser-assisted processing of the electrode/electrolyte interphase aims to create a 3D morphology by opening channels that facilitate faster electrolyte diffusion, hence enhancing charge/discharge rates. While such studies have primarily focused on battery electrodes, these improvements are critical for the development of high-performance supercapacitors designed for energy storage applications that require rapid energy delivery and long operational lifetimes [2].

This work explores how laser-assisted microstructure modification influences the performance of electrodes. Various laser fluences have been utilized to modify the structure and morphology of slurry-based activated carbon electrodes prepared using the conventional doctor-blade coating method. A 3D imaging technique in Photoshop, based on creating channels to detect subtle variations in morphology and perform measurements of the area of interest, has been developed to characterize the porosity of modified electrodes in comparison to untreated electrodes. This technique appears more favorable as it reduces human intervention in calculations compared to the thresholding approach [3]. The surface area is determined using the Brunauer–Emmett–Teller (BET) method.

Tortuosity factor is obtained through numerical modeling of diffusion transport inside microporous structure. A combination of X-ray Computed Tomography (XCT), a non-destructive method capable of analyzing larger structures, and Focused Ion Beam Scanning Electron Microscopy (FIB-SEM), which offers higher resolution, provides comprehensive insight into electrode morphology [4]. The 3D reconstructions obtained from these techniques are used to develop numerical models for steady state diffusion inside a free space control volume and comparing it with diffusion transport through pores (in the actual structure). Additionally, a “zoom-in” approach (a window within another window) is adopted to bridge the different length scales investigated by XCT and FIB-SEM. This hierarchical modeling method provides a more accurate representation of the complex pathways for ion and electron transport, aiding to identify bottlenecks and heterogeneities within the porous medium that affect performance.

By correlating structural parameters with transport properties, the study aims to provide design guidelines for optimizing electrode architecture. The integration of imaging and modeling techniques contributes to the development of next-generation supercapacitor electrodes with improved efficiency, higher power density, and enhanced long-term stability.

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References:

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MS01 / 374

Methodological considerations to assess biogeochemical reactivity during hydrogen storage in a carbonate aquifer

Author: Soetkin Barbaix¹

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Underground Hydrogen Storage (UHS) is emerging as a promising technology to enable large-scale and efficient storage of renewable energy, addressing the challenges of renewable energy intermittency and decarbonization. Carbonate host rocks, albeit representing one quarter of the potential UHS storage sites in Europe, have only recently started to receive attention in literature. One of the reasons being their potential increased reactivity compared to more inert sandstone host rocks and salt caverns. However, dynamics and kinetics of both geochemical and microbial reactions, and especially their relationship, remain unclear.

This study focuses on evaluating the effects of biogeochemical processes and their interplay on UHS in fractured carbonate saline aquifers, with a case study in Loenhout, Belgium. Low and high pressure batch reaction experiments are conducted to investigate the interactions between hydrogen, the natural brine, the subsurface microbial community, and mineral phases (pyrite-containing limestone) under reservoir-relevant conditions. This brings along unique challenges related to the extreme nature of the reservoir and the unique organisms that are found. Key parameters such as gas composition, microbial community composition and composition of the liquid phase are monitored to assess activity and its impact on UHS.

Preliminary results indicate low initial cell counts, with communities mainly comprising sulfate reducing bacteria, and slow kinetics for both growth and metabolic activity. For the geochemical experiments, the first results show no measurable activities. These findings provide valuable insights into the complex reaction dynamics of UHS in carbonate reservoirs.

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MS11 / 375

Rock microfluidics under pressure: enabling geochemical observations at subsurface conditions

Author: Wen Song¹

¹ *University of Texas at Austin*

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Real-rock microfluidics have enabled elucidation of *in situ* fluid-rock interactions at the fundamental scales of length and time ($\sim \mu\text{m}$, ms). These platforms are categorized broadly into three classes: those constructed from rock material (e.g., calcite, shale) that are pressure-constrained by the mechanics of the crystal substrate, those deposited with mineral particulates (e.g., kaolinite, brucite, etc.) that lack spatial control and realism, and those precipitated with minerals *in situ* that are limited to systems with fast reaction kinetics. Microscale resolution of geochemical interactions in decarbonization-critical lithologies such as basalts at realistic subsurface conditions, as a result, remain inaccessible. In this talk, I will show a new platform that enables, for the first time, the direct observation of geochemical interactions within natural mafic matrices at elevated pressures and temperatures representative of subsurface environments. Interfacial reactions are characterized for mono- and di-mineralic systems to understand the nonlinear influence of secondary species on overall reaction kinetics.

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MS24 / 376

Molecular dynamics study of swelling of wood-inspired polymeric composite and other interactions with water

Authors: Ali Shomali¹; Wenqiang Liu^{None}

Co-authors: Eleanor Schofield²; Benoit Coasne²; Jan Carmeliet³; Dominique Derome⁴

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We study the hygro-mechanical behavior of composite consisting of amorphous cellulose, xylan, lignins reinforced or not with crystalline cellulose and treat the composites with polyethylene glycol as consolidant. We simulate water adsorption and desorption in amorphous polymers, allow observations on mechanical behavior like swelling and shrinking, mechanical softening in compression and shear, and on the stick-slip behavior of the stiff fibrils pulled out of the matrix. To better understand the hygro-mechanical behaviour of biopolymer composites upon sorption and desorption, Molecular Dynamics combined with Grand Canonical Monte Carlo simulations [\[1\]](#) is used to study sorption-induced deformation and determine the mechanical properties of wood-inspired biopolymer composites and a system approaching S2 configuration.

Atomistic modeling is an insightful tool for the in-depth study of the coupled effects of water sorption on hygric and mechanical properties of different polymeric components. Molecular modeling can contribute to support and complement experimental methods which yield, most frequently, indirect structural information. With molecular modeling, there is a freedom of investigating unlimited possibilities of configurations, ranging from individual wood polymer materials to composite structure resembling subunits of wood S2 cell wall. We present recent insights on wood cell wall S2 layer hygromechanical behavior [2](#).

Composites show swelling-induced sorption and a mechanical weakening upon sorption. Due to the reinforcing effect of the crystalline cellulose fibre, the swelling and weakening of composites in longitudinal direction is suppressed. Additional sorption is found to occur in the porosity created by the misfit between crystalline cellulose fibre and matrix, leading to a reduction of the pullout shear strength due to breakage of matrix-fiber hydrogen bonds by the water molecules. Adding polyethylene glycol to composites results in filling the gap between crystalline cellulose and matrix, leading to a reduction of the volumetric swelling and sorption, and an enhancement of the pullout shear strength.

We observed hysteresis not only in water sorption but also in mechanical properties. This hygromechanical behavior can also be observed in particular from the breaking and reforming of hydrogen bonds.

This work is inspired by wood, an orthotropic cellular biomaterial, and by treatment of waterlogged archaeological wood of shipwrecks, like the Varsa and Mary Rose, with PEG for its consolidation and stabilization, where PEG molecules replace the water making wood at museum conditions less susceptible to changes in humidity and able to sustain mechanical load.

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Student Awards:

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MS03 / 377

Bridging the gap between field observations and modeling of fracture networks

Author: Matthew Sweeney¹

Co-authors: Hari Viswanathan ¹; Jeffrey Hyman ¹

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Despite the amount of research on flow and transport in single fractures and fracture networks, there is a gap in knowledge between the field data describing natural fractures and the models that represent them. Natural fracture networks exhibit ranges of fracture lengths, connectivity, and aperture distributions, which directly affect the flow and transport behavior within the network. The values

for these parameters are related to the formation conditions for the fractures themselves, whether from mechanical, chemical, or thermal processes, or some combination thereof. In numerical models of fracture networks, values for these parameters are commonly assumed based on statistical distributions or are stochastically generated. This is typically done under the guise of theoretical considerations, meaning the actual values are secondary to the phenomenology and quantities of interest under study. However, some field data indicate that apertures do not follow well-defined statistical distributions, particularly in sedimentary rocks that have undergone diagenesis. If certain fractures are cemented in the network, the flow and transport behavior can be expected to vary because connectivity can be reduced. Incorporating such effects into numerical models has only been done for simple cases in three-dimensions and the effects of such aperture changes have not been systematically investigated or linked to other fracture network characteristics or high-fidelity flow and transport simulations. Therefore, it is critical to understand when typical modeling assumptions might fail to accurately predict flow and transport in natural or engineered fractured systems. In this work, we investigate how model assumptions that neglect rock specific aperture data might impact flow and transport through fracture networks. Specifically, we have incorporated the concept of the emergent threshold, or the characteristic length scale above which fractures will flow, into discrete fracture network models and performed high fidelity flow and transport simulations based on both field and stochastically generated aperture and fracture length data. Changes in emergent threshold can alter the flow structures within the networks by closing existing preferential pathways and lowering effective permeabilities, which in turn can increase flow channeling in the networks, but these effects are closely linked to the underlying network structure (i.e., topology) and density, as well as the matrix permeability. Our results indicate that emergent threshold/fracture sealing can be a first order control on network scale flow and transport and further motivates future work linking additional field observations to numerical models of fracture networks.

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MS06-B / 378

Quantifying Voidage Distributions in Fluidised Bed Reactors Using CFD-DEM Simulations

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In drinking water purification operations, liquid-solid fluidised (LSF) bed reactors are often used, for example in seeded crystallization softening processes (1). Fluidised beds can be considered as dynamic porous media with fascinating spatio-temporal behaviours (1). Usually, LSF systems are considered to be homogeneous under moderate superficial fluid velocities. However, recent fluidisation experiments using calcite grains have demonstrated the appearance of discrete water “pockets or parvoids” at low superficial liquid velocities, evolving into more complex structures at higher velocities (1). It remains unclear however, whether such heterogeneous behaviour benefits or hinders

the chemical crystallization efficiency (2,3).

Based on the results presented in (1), we extend the Computational Fluid Dynamics - Discrete Element Method (CFD-DEM) simulations to obtain more detailed information about the observed heterogeneous behaviour (2,3). Simulations are performed using different water inlet velocities and different calcite grain size fractions obtained from full-scale reactors. We analyse our results in terms of voidage and particle distribution functions. Images of the experiments and simulations are visually compared for the formation of voids, see Fig.1. The simulations show clear differences in void fraction for different flow rates in the cross-section of the column. The heterogeneity and onset of fluidisation behaviour obtained from the simulations and experimental observations are found to be in statistically significant agreement. Finally, for particle sizes smaller than reported in (1), we find that the range of observed voidages is much narrower compared to using larger particles.

This clearly demonstrates that voidage must not be assumed as a single constant value. Instead, LSF beds shows significant spatial and temporal variations with distinct regions of higher and lower voidage, forming dynamic structures throughout the bed. This finding is critical as it underscores the need to move beyond simplified homogeneous models when analysing and designing fluidised bed systems. Accounting for these distributions offers a more accurate representation of the system's behaviour, which could lead to improved predictions of hydrodynamic performance and enhanced optimisation of processes such as crystallisation in water softening reactors.

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MS01 / 379

Experimental Investigation of Mudrock Capillary Sealing and Re-sealing to CO₂

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Structural trapping of buoyant fluids, including carbon dioxide (CO₂), depends on the caprock capillary and mechanical sealing capacity. The capillary sealing capacity of mudrocks depends on rock

composition, fabric, dynamic drainage and imbibition processes, pressure and temperature, among others. The objectives of this study are (1) to evaluate potential changes of breakthrough pressure at reservoir pressure and temperature, and (2) to measure snap-off pressure after breakthrough. The study uses resedimented kaolinite in brine and is divided into two main sections: capillary breakthrough experiments at pressures between 25 and 42 MPa and temperatures between 60°C and 80°C using the step-by-step differential pressure increase method, and snap-off pressure measurements using the residual capillary pressure method. The results show (1) positive breakthrough pressures to displace brine with CO₂ which remain in the same range of 1.4 to 2.8 MPa, and (2) average post-breakthrough relative permeability of 5% for all tested pressures and temperatures. The snap-off experiments results show differential capillary pressures ranging from 0 to ~1.4 MPa. The differential pressure at snap-off depends on the initial CO₂ mass upstream. Overall, the results show that kaolinite mudrocks are satisfactory barriers for CO₂ by development of capillary forces and brine re-imbibition in case drainage by CO₂ occurs. Both processes are possible due to the water-wet nature of kaolinite clay. The results can be extended to other clays typically found in naturally occurring seals.

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Poster / 380

OPTIMIZATION OF GEOLOGIC CARBON SEQUESTRATION: EFFECT OF FLOWRATE ON NONWETTING PHASE CONNECTIVITY.

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Reducing atmospheric carbon is essential in the global strategy to combat climate change. The International Panel on Climate Change's Fifth Assessment Report emphasizes the critical goal of keeping the rise in global temperatures to under 1.5°C compared to pre-industrial levels. The report highlights that achieving this temperature goal is unlikely without proper deployment of counteractive emission strategies such as carbon capture, utilization, sequestration, and storage (CCUS). Geological carbon sequestration, primarily via the residual trapping mechanism, is a workable approach for efficiently storing CO₂ in subsurface formations over comparatively short geological periods. However, careful management of the trapping efficiency is crucial to provide optimal CO₂ storage.

According to exploratory research of limited scope (Davis, 2021), reducing the topological connectivity of CO₂ within subsurface formations may improve the effectiveness of residual trapping. These preliminary findings demonstrated a correlation between increased CO₂ injection flow rates and a reduction in nonwetting phase connectivity, suggesting that higher flow rates may enhance capillary trapping. The purpose of this study was to further examine the effects of different drainage flow

rates on nonwetting phase connectivity, which could optimize trapping efficiency, ultimately resulting in better CO₂ retention. Proxy fluids represented nonwetting and wetting phases, with Soltrol 220® and water as the analogs for supercritical CO₂ and subsurface brine. The study further focused on flow rate-dependent changes in fluid connectivity after injection to identify flow conditions that result in the most efficient residual trapping.

Experiments were conducted under variable drainage flow rates while using a sintered glass bead column, a widely recognized model for porous media. X-ray computed microtomography (micro-CT) was used to capture detailed three-dimensional images of fluid distributions. Imaging was performed at four critical stages: before fluid injection, after the primary imbibition, post-drainage, and after secondary imbibition. Image analysis then allowed for the extraction of connectivity metrics, precisely the Euler number, and phase saturations to evaluate the changes in fluid connectivity and trapping efficacy.

This work provides valuable insights into flow dynamics that could be used to fine-tune geologic carbon sequestration techniques, leading to improved CO₂ storage strategies. Ultimately, optimizing CO₂ trapping efficiency holds great potential for enhancing the overall effectiveness of CCUS, contributing to the multidisciplinary approach needed to combat climate change.

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References:

Davis, B. (2021). Optimization of Geologic Carbon Sequestration: Effect of Flowrate on Nonwetting Phase Connectivity, MS thesis, Oregon State University. https://ir.library.oregonstate.edu/concern/graduate_thesis_or_dissertation

Poster / 381

Extending the reach of microbes in precipitating carbonates for geologic gas storage

Author: Wen Song¹

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Geologic gas storage opens exciting horizons for at-scale decarbonization (e.g., CO₂ storage, seasonal H₂ storage, etc.), but is encumbered by potential for leakage due to fluid-solid reactions (e.g., embrittlement, permeability heterogeneity). The distribution and control of naturally-occurring bacteria that enable mineralization in these formations, a process known as microbially-induced carbonate precipitation (MICP), provides an opportunity to heal storage formations *in situ*. Practical implementation of MICP in the field, however, is challenged by poor control over the spatial extent of carbonate precipitation, where carbonates are precipitated primarily within ~ cm of the injection site. In this talk, we investigate the reactive transport controls on MICP necessary to enable deep MICP penetration into the formation using porous micromodels. Specifically, we show that cation-assisted microbe adsorption on pore surfaces enables uniform microbial distribution across

the porous medium rather than local accumulation near the inlet, and extends the spatial reach of MICP throughout the pore space.

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MS09 / 382

Characterizing the Morphology and Permeability of Multiscale Pore System of Carbonate Rocks

Authors: Ingrid Bertin Carneiro¹; Celso Peres Fernandes¹

Co-authors: João Pedro Tauscheck Zielinsk²; Anderson Camargo Moreira¹; Iara Frangiotti Mantovani¹

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The pore structure of carbonate rocks is intrinsically heterogeneous, with pore sizes ranging several length scales due to the depositional and diagenetic processes. It strongly influences the morphology and connectivity of the pore system and the petrophysical properties of these rocks. Because of this multiscale characteristic, the pore network characterization and the prediction of macroscopic properties remain challenging. In the past two decades, digital rock analysis (DRA) has gradually become an important approach for permeability (and other rock properties) prediction. Indeed, using X-ray imaging techniques and numerical modelling, it is possible to estimate petrophysical properties in 3D microtomography images using fundamental physical equations applied to the pore scale. Beyond estimating properties in representative elementary volumes (REV) of the rock, this approach can improve our knowledge of the relationship between properties and pore structure. This work implements a workflow including laboratory experiments, image acquisition and processing, and analysis to characterize the multiple porosities of samples of Coquinas from Morro Do Chaves formation (CIMPOR Quarry outcrop, São Miguel dos Campos, Alagoas, Brazil). A central aspect of the workflow is the data integration obtained from entire core-plug and sub-samples micro-CT images and mercury intrusion capillary pressure (MICP) measured at core-plug subsamples, aiming for a more accurate estimation of the absolute permeability. The images acquired by X-ray microtomography are limited to a voxel size of about 1 mm; in general, a significant fraction of the pore volume is below this size and is not clearly defined (or resolved). In our workflow, the MICP data supply the description of the sub-resolution porosity; do not consider this sub-resolution porosity can lead to underestimated permeability values. The Stokes-Brinkman equations modelled the single-phase fluid flow in the pore space, including the sub-resolution porosity. This hybrid model solves the Stokes equations in the resolved pore regions and Darcy's law in the sub-resolution regions. Applying the present workflow to Morro Do Chaves's samples demonstrates the importance of a multiscale treatment of these rocks using appropriate analysis techniques for each spatial scale. The rock permeability results are related to the size distribution and connectivity of the pore network of each scale.

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MS03 / 383

Learning the factors controlling mineral dissolution in three-dimensional fracture networks

Author: Aleksandra Pachalieva¹

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We perform a set of high-fidelity simulations of geochemical reactions within three-dimensional discrete fracture networks (DFN) and use various machine learning techniques to determine the primary factors controlling mineral dissolution. The DFN are partially filled with quartz that gradually dissolves until quasi-steady state conditions are reached. At this point, we measure the quartz remaining in each fracture within the domain as our primary quantity of interest. We observe that a primary sub-network of fractures exists, where the quartz has been fully dissolved out. This reduction in resistance to flow leads to increased flow channelization and reduced solute travel times. However, depending on the DFN topology and the rate of dissolution, we observe substantial variability in the volume of quartz remaining within fractures outside of the primary subnetwork. This variability indicates an interplay between the fracture network structure and geochemical reactions. We characterize the features controlling these processes by developing a machine learning framework to extract their relevant impact. Specifically, we use a combination of high-fidelity simulations with a graph-based approach to study geochemical reactive transport in a complex fracture network to determine the key features that control dissolution. We consider topological, geometric and hydrological features of the fracture network to predict the remaining quartz in quasi-steady state. We found that the dissolution reaction rate constant of quartz and the distance to the primary sub-network in the fracture network are the two most important features controlling the amount of quartz remaining. This study is a first step towards characterizing the parameters that control carbon mineralization using an approach with integrates computational physics and machine learning.

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Modeling and Simulation of NMR-Based Pore Size Distribution in Porous Media

Author: Sinai Morales Chavez¹

Co-authors: Everton Lucas-Oliveira²; Martín A. Díaz-Viera¹; Miguel A. Valdéz-Grijalva¹; Tito J. Bonagamba³

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Nuclear magnetic resonance (NMR) is a valuable technique for studying porous media. Through the measurement of transverse relaxation times (T_2), which are directly related to pore size, NMR allows the estimation of critical parameters such as porosity, permeability and fluid type. In porous media that exhibit a distribution of pore sizes, T_2 typically consists of a superposition of multiple exponential decays, obscuring the underlying pore characteristics. Therefore, despite being a mathematically ill-posed problem, the Inverse Laplace Transform (ILT) is the most common approach to obtaining T_2 values from multi-exponential decay signals. After ILT, it is possible to determine pore size distribution (PSD) and identify fluids occupying pores.

In recent years, NMR has received considerable attention for the study of porous materials in various industries, including groundwater exploration^[1]. Extensive research has shown that NMR provides valuable insight into fluid-rock interactions and the morphology of porous media [2, 3]. Numerous studies have attempted to characterize porous media by correlating the T_2 distribution from NMR data with the PSD and comparing these results with other experimental techniques (e.g. capillary pressure test, mercury intrusion porosimetry or micro-computed tomography) [4, 5, 6]. However, these studies often rely on simplifying assumptions, in particular neglecting the effect of transverse bulk relaxation (T_{2B}) of the fluid, which can lead to significant underestimation of pore size [7].

Numerical simulation offers another approach to PSD analysis, in particular the Finite Element Method (FEM) offers remarkable computational flexibility for modeling simple geometries, such as spherical shapes, using coordinate transformations and exploiting geometric symmetry to reduce the DOF while maintaining a comprehensive representation of the physical phenomenon and improved computational efficiency.

This work proposes a simplified mathematical NMR model and numerical implementation based on FEM to simulate transverse magnetization signals for a PSD, validated by comparing the numerical solution with semi-analytical solution, and introduces a novel variable change in the ILT to convert T_2 distributions into a PSD. The numerical model is developed using FEM, and the results are validated by comparison with semi-analytical solution considering the effect of T_{2B} . Application cases in synthetic porous media and Berea sandstone are presented, showing a favorable correlation between experimental and simulated data.

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MS15 / 385

Learning to Simulate Flow through Porous Media with Graph Neural Networks from Experimental Data

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Fluid flow in porous media plays a crucial role in many environmental and energy sciences applications, including groundwater management, hydrogen and carbon storage, and fuel cells. However, the numerical modeling of such processes remains a very challenging task. Traditional numerical simulation methods often struggle to rapidly and accurately predict pore-scale flow processes in porous media due to high computational costs, complex mesh generation, and difficulty capturing nonlinear flow behavior. To address these challenges, we explore a new modeling framework based on graph neural networks to learn the flow process from experimental data directly. We developed a Pore-scale Graph Network Simulator (Pore-GNS), which embeds pore-structure information in graph construction and introduces soft physical constraints to assist learning. This approach effectively captures the impact of confined spaces on fluid flow while accurately predicting the dynamic evolution of flow fields. By leveraging experimental data of fluid particles for learning, our method can produce particle trajectories for unseen periods and corresponding velocity fields.

Our approaches use real particle motion data obtained from fluid flow in actual porous media as training and validation datasets. The results demonstrate that the Pore-GNS predictions are highly consistent with those from the datasets. Moreover, predicting the single-step trajectories of nearly 1,000 particles takes less than 10 seconds, and generating complete and reliable velocity fields through multi-step autoregressive inference requires only a few minutes, significantly reducing computational overhead. This method shows strong potential for rapid flow prediction in porous media, providing a more efficient solution for geological reservoir simulation, environmental monitoring, and water resource management. As the model scale and multiphysics coupling continue to expand, this approach provides a promising direction for future porous media flow modeling.

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386

Experimental Investigation on Illite Clay for Sustainable Ground Stabilization

Author: Rene Tammen¹

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Quick clay is a highly sensitive type of clay formation that can liquefy when disturbed, leading to catastrophic and deadly landslides in Norway, USA, Canada, Sweden, and Finland. To stabilize these areas, lime-cement is commonly used. This method is relatively simple and inexpensive, however the significant drawback is a large CO₂ footprint. To explore a more sustainable stabilization, our project "Sustainable Stable Ground" investigates the quick clay formation from an atomic scale and upscale to geological scale.

In this presentation, I will focus on our experimental investigation of Illite suspensions, the primary clay mineral in quick clay, under various conditions, including different ionic strengths and the addition of diverse (sustainable) additives. Our studies included experimental analysis of the Tiller-Flotten quick clay from the Trondheim area in Norway, as well as the use of purified clays for controlled experiments.

To characterize the physical and chemical properties of the clay, we employed various methods, including Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), zeta potential measurements, and rheology. We tested different salts, such as NaCl, MgO, KCl, and others, observing that higher salt concentrations led to a more stable system. Additionally, we initiated tests with various hydroxide and polymers. Our objective is to identify potentially sustainable stabilizers by creating different suspensions with diverse (eco-friendly) additives, allowing for long-term observation of the clay-rich ground.

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MS13 / 387

Experimental investigations of H₂, He, CH₄ and CO₂ adsorption, wettability and geomechanics on kerogen at geo-storage conditions

Author: Bin Pan¹

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Kerogen is the most abundant form of organic matter in the subsurface and its properties of adsorption, wettability and geomechanics affect gas (H₂, He, CH₄ and CO₂) geo-storage (GGS) capacity and leakage risk. However, a systematically experimental investigation of these three properties at in-situ GGS conditions is lacking and thus large uncertainties exist in evaluating the impact of kerogen content on GGS integrity. Therefore herein, kerogen properties were investigated experimentally at GGS conditions, based on isothermal adsorption, contact angle, and nanoindentation measurements. It is demonstrated that 1) the maximum adsorption capacity for H₂, CH₄ and CO₂ is 0.3789 mol/kg, 3.5360 mol/kg, and 5.2625 mol/kg respectively (occurring at various thermophysical conditions), thus following the order H₂ < CH₄ < CO₂; 2) kerogen wettability ranges from weakly water-wet to gas-wet with its affinity to gases following the order He < CO₂ < H₂ < CH₄; and 3) after exposure to H₂, He, CH₄, liquid CO₂ and H₂O for 3–5 mins, the Young's modulus of kerogen decreases by 45%, 32%, 1%, 70%, and 50% respectively, while the kerogen pellet disintegrates after exposure to supercritical CO₂ for 3 mins. This study provides key data for evaluating GGS, an important pathway for accelerating the energy transition, promoting the advanced technology development, balancing the energy supply and demand, and mitigating the carbon emissions.

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MS08 / 388

Contribution of soil structure and colloidal particles to the leaching of PFAS in undisturbed soil columns

Author: Elisabeth FRIES^{None}

Co-authors: Beatrice BECHET¹; Chloe CAUREL; Denis COURTIER-MURIAS; Eric MICHEL; Helene BUDZINSKI; Pierre LABADIE; Pierre-Emmanuel PEYNEAU¹

¹ *Université Gustave Eiffel*

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The term 'per- and polyfluoroalkylated substances' (PFAS) refers to a broad class of molecules containing at least one perfluorinated methyl (-CF₃) or methylene (-CF₂-) group¹. Their properties have led to their use in a large number of applications since the 1940s. Unfortunately, they are persistent in the environment or metabolised into persistent substances, bioaccumulative and harmful to ecosystem health.

Soil plays a key role in the fate of PFAS: it delays their arrival in aquifers and allows them to be internalised by crops and biota. Since 2009², the transport of PFAS in soils has been studied by lab experiments, mainly in model soils: columns filled with sand or crushed and recompact soil, saturated with water and artificially contaminated with one or more molecules. These experimental situations have limitations because: (i) soils are often contaminated by mixtures of PFAS³, which can lead to competitive adsorption phenomena; (ii) in situ, PFAS are present in soils for years, allowing slow processes to affect their fate^{6,7} (e.g., metabolism, transport to the microporosity by diffusion or during humidification/drying cycles); (iii) two modes of transport in structured soils have not been considered: (a) transport as colloidal phase, facilitating the mobility of molecules with a strong affinity for the soil constituents and which would otherwise have little mobility⁸. This mechanism could contribute to the mobility of long-chain PFASs, interacting strongly with organic matter, which is itself assumed to be immobile; (b) preferential transfer into the largest porosity in the soil (macropores linked to the action of soil fauna or roots), facilitating the vertical transfer of PFAS present in the colloidal or aqueous phase.

The mechanisms that determine the fate of PFAS in the experimental situations studied so far are not necessarily the same as those under field conditions. We have explored these in situ mechanisms by considering a more realistic experimental situation: simulated rainfall on columns of undisturbed soil from a former firefighting training site, contaminated by a cocktail of molecules.

The X-ray tomography reveals the diversity of pore size and connectivity even at column scale, mainly contributing to the hydrodynamics during rainfall (preferential flow and/or predominantly matrix flow, even ponding). These experiments showed that (i) the hydrodynamic conditions, linked to soil structure, had a moderate influence on the extent of colloidal-phase transport of PFASs, more related to the location on the hydrograph, (ii) when the perfluorinated chain length n_c was ≤ 7 , diffusion was the mechanism limiting transport, (iii) colloidal particles facilitated the mobility of certain fluoro-telomers and perfluorinated acids with $n \geq 8$, so far only shown with PFOA in model soils⁵. These results enabled us to refine the conceptual model of the fate of PFASs in soil and to propose the mechanisms that should be studied to improve it. Competitive sorption phenomena - rarely studied in soils - could be a mechanism that should not be overlooked in understanding the transport of PFAS in mixtures.

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MS07 / 390

Numerical Modeling of CO₂ Solution Injection into Korean Basalt for Rapid Geological Carbon Storage through Mineralization

Authors: Soeun Yoon¹; Baehyun Min¹

Co-authors: Youngbin Ahn ¹; Tae-Hyuk Kwon ²; Jeonggyu Seo ³; Jaehan Park ³; Jihyuk Kim ³; Hosang Kim ³

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CO₂ storage in basaltic formations has emerged as a promising method for carbon sequestration due to its rapid mineralization rates, as demonstrated by several projects (e.g., CarbFix in Iceland, Wulula in the USA, and 44.01 in Oman). This study numerically investigates the efficacy of CO₂ solution injection into basalt formations in the Republic of Korea. We implement geochemical reactions for basalt dissolution and carbonate precipitation, accounting for changes in porosity and permeability. The model's performance is validated by comparing core-scale simulation results with experimental data from CO₂-ionized water injection into basalt outcrop samples from Cheorwon and Jeju Island, volcanic regions in Korea. Performance evaluation criteria include calcite precipitation, porosity, permeability, and pressure changes. Sensitivity analysis examines the effects of CO₂ solution types (i.e., CO₂-ionized water vs. CO₂-dissolved water) and mineral compositions on carbon mineralization. Following the core-scale analysis, we conduct field-scale simulations of CO₂ solution injection using geophysical data of basaltic formations near Jeju Island. The field-scale study examines the contributions of solubility trapping and mineral trapping mechanisms under various storage conditions, including depth, temperature, pressure, and fracture density. Furthermore, the effects of CO₂ concentration in the injected fluid are analyzed to identify efficient and secure carbon sequestration strategies that minimize leakage risks. These modeling and simulation results provide insights into the potential of CO₂ storage in Korean basaltic formations, contributing to the country's carbon capture and storage initiatives.

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Poster / 392

Optimizing Operational Parameters for PFAS Permeable Reactive Barrier Emplacement

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Perfluoroalkyl and poly-fluoroalkyl substances (PFASs), as constituents of many industrial products, pose significant risks to groundwater quality and ecosystem health due to their persistence in the environment and their association with various health issues. Permeable reactive barriers (PRBs)

can offer a cost-effective and energy-efficient in situ solution for PFAS groundwater plume remediation by passively retaining and/or breaking down contaminants when installed across the flow path. Polymer-stabilized activated carbon (S-PAC) nanoparticles (NPs, which can be injected directly into a contaminated formation, are among the most effective and economical barrier materials for PFAS retention.

Here, a radial mathematical model for S-PAC field emplacement is presented and employed to explore operational factors that can affect barrier performance in the field for effective sorption of two representative PFAS, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS), both of which have a maximum concentration limit (MCL) of 4 ppt. Wurtsmith Air Force Base (Michigan, U.S.) is used as a representative case study for barrier installation. The model is based on modified filtration theory (MFT) and demonstrated to reproduce the observed behavior of S-PAC delivery in packed column bench-scale experiments. Column-fitted parameters are employed to investigate the sensitivity of barrier retention behavior to NP attachment parameters and operation injection parameters. Here, a pseudo-first-order kinetic model, based on a Freundlich isotherm, is implemented to model sorption. The target of the optimization process is to maximize the longevity of the barrier, defined by the time required for concentration breakthrough at a level that exceeds the MCL; while the total operation time, the total injected mass of NPs, and the well-spacing are fixed to ensure the greatest possible longevity of the barrier within the same cost. The retention of NPs within a range of attachment rates (k_{att}) and maximum attachment capacities (S_{max}) were modeled to find the best set of pumping rates and injection concentrations that leads to the greatest barrier longevity for different sorption rates.

Simulation results indicate that high k_{att} and low S_{max} generally lead to significant nanoparticle retention for multiple injection strategies. However, for low k_{att} and high S_{max} , the retention profile depends more on the operational parameters (such as pumping rate and injection concentration). For these cases, a push-pull strategy is proposed to achieve a barrier with greater longevity. The proposed push-pull strategy is particularly effective in non-ideal situations where k_{att} is low, offering a significant advantage over the conventional push scenario. This research highlights the importance of choosing the proper operational parameters to design a long-lasting PRB for treating PFAS-contaminated groundwater.

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Poster / 393

Experimental investigation of hydrogen and cushion gas mixing during underground hydrogen storage in porous reservoirs

Author: Ianna Gomez Mendez¹

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Hydrogen has gained interest in recent years as a clean energy source and form of energy storage to support renewables. Porous underground reservoirs (e.g., saline aquifers and depleted gas reservoirs) could accommodate the high volumes of safe, long-term storage that will be needed to support

hydrogen economies but remain unproven for underground hydrogen storage (UHS). In particular, cushion gas must be present in such reservoirs to assure brine displacement and pressure maintenance during the hydrogen withdrawal stage. However, the mixing between hydrogen and the cushion gas in the porous media decreases the purity of the gas withdrawn. Understanding how this mixing occurs in porous media and which parameters can help control it is critical to assessing the viability of UHS in various porous geologic reservoirs. In this work, a miscible core flooding experiment of hydrogen displacing supercritical carbon dioxide (as cushion gas) is conducted to estimate the dispersion coefficient from the fitting of the convection-dispersion equation with the experimental breakthrough curve. A Gray Berea sandstone core (2 in. diameter by 6 in. length) is initially saturated with supercritical carbon dioxide (CO₂) at 40°C and 1500 psi of pore pressure, which is displaced by hydrogen gas at a fixed flow rate supplied by a syringe pump. The hydrogen concentration in the binary mixture gas is measured by a portable gas analyzer and is corroborated by the results of gas samples analyzed in a Gas Chromatograph Mass Spectrometer. This cycle of experiments is repeated for a range of flow rates that varies from 0.1 ml/min to 10 ml/min. The dispersion coefficients are calculated for each flow rate. Resultant data provides needed inputs for UHS field simulations as it represents relevant reservoir conditions and the complexity of supercritical CO₂ as cushion gas. Understanding mixing and displacement phenomena in porous media is necessary to evaluate feasibility and optimize operations of UHS in porous reservoirs of interest.

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MS25 / 394

Towards relative permeability-mineralization paradigms in vesicular basalt pore systems

Author: Shaina Kelly¹

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This talk discusses pore-scale controls on multiphase flow in vesicular basalts for carbon storage and mineralization processes. Multiphase flow adds an additional mass transfer step across brine-CO₂ phase boundaries and spatially impacts reactant mixing paths, mineral (e.g., carbonate) growth patterns, and relative permeability during supercritical CO₂ injection. Ergo, consistent quantification of CO₂-accessible pore systems and reactive mineral surface area in basalts (and other mafic/ultramafic rocks) as a function of partial water saturation state (*S_w*) and flow regime is critical for effective carbon storage and mineralization. However, unlike conventional rocks, there are no established paradigms for basalt capillary-pressure (*P_c-S_w*) and relative permeability (*K_r-S_w*) relationships. These relationships are challenged in basalts due to their unconventional nanoporous and/or dual-porosity pore systems and complex primary and secondary (altered) mineral assemblages. First, this work identifies basalt pore and mineral (primary and secondary) microstructures as a function of alteration with combined optical microscopy, SEM/EDS, microCT, NMR, BET, and gas pycnometry techniques and relates these to *P_c-S_w* paradigms. The study highlights microstructures from subsurface

vesicular basalt samples of varied alteration states from carbon mineralization and geothermal exploration projects (e.g., Columbia River Basalts, Newberry Volcano, American Samoa). Quantified microstructure includes grain fabric assemblages (e.g., phenocrysts, glass, and alteration clays), pore morphology (e.g., surface roughness, tortuosity), and pore-facing mineral surfaces. Next, brine-CO₂ or brine-non-wetting phase distributions within subsets of the aforementioned pore systems are probed through a combination of computational fluid dynamics (CFD, lattice Boltzmann method), dual-porosity microfluidic proxy work, and imbibition data. Previous CFD work by the authors in collaboration with Pacific Northwest National Lab have revealed that partial saturation states are a control on engineered carbonate growth at PNNL's Wallula Basalt Injection Pilot. This work further probes phase distributions in dual-porosity microstructures (nanopores and micro-to-macropores) through flow rate and S_w states, whereby low S_w values are thin film regimes, $S_w = 1$ is single phase flow, and immediate values are capillary flow and bubble regimes. While the representative elementary volume (REV) for basalts remains uncertain, insights from these combined static and dynamic analyses reveal the major impacts of alteration state, pore to throat aspect ratio, pore size distribution, and connectivity on brine-CO₂ phase distributions in vesicular basalt pore systems. Finally, we discuss implications and next steps towards relative permeability curves in vesicular basalt for optimized carbon mineralization.

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Poster / 395

Impacts of Accessible Surface Area on CO₂ Mineralization in Basalt Formations

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As global warming intensifies, CO₂ sequestration has been recognized as one of the most feasible strategies for reducing CO₂ emissions. Within CO₂ sequestration approaches, the CO₂ mineralization process, a promising CO₂ sequestration method, consists of four main steps: (1) injection of CO₂-saturated water into basalt formations, (2) dissolution of mafic minerals within the porous media, (3) release of divalent cations (Ca²⁺, Mg²⁺, Fe²⁺) into aqueous phases, and (4) precipitation of carbonate minerals, thereby immobilizing CO₂ as stable solid phases. To evaluate the CO₂ mineralization capacity in basalt formations in relation to fluid accessibility, numerical simulations were conducted for the CarbFix project site and the Jeju basalt formation based on comprehensive analyses. The physicochemical properties of two basalt samples were characterized through detailed petrophysical and geochemical analyses. Porosities and permeabilities were quantified using micro-CT imaging and

MICP porosimetry. Primary mineral compositions were identified as albite, anorthite, diopside, hypersthene, alkali feldspar, forsterite, fayalite and ilmenite through XRD, EPMA and whole-rock analysis. The kinetic parameters of mineral reactions are crucial factors during the CO₂ mineralization process. Among the kinetic parameters, the mineral reactive surface area, a site-specific property, has a predominant impact on the reaction rate of mineral dissolution/precipitation. In early studies, reactive surface area was employed as specific surface area (SSA), which represents geometric surface area of mineral particles per unit mass. Recent geochemical studies suggest adopting the accessible surface area (ASA), which quantifies the accessibility of minerals to reactive fluids within porous media, to better account for heterogeneous reactions. To investigate the impact of fluid accessibility on CO₂ mineralization through numerical simulation, SSA and ASA were quantified through SEM image analyses and utilized as input parameters in numerical simulations. Numerical simulations were performed over a 100-year period, with CO₂-saturated water (1 mol/kg) injected for the first 5 years at a rate of 100 kg/s. The simulations evaluated the long-term effects of SSA and ASA on CO₂ mineralization in basalt formations. Over 90% of the injected CO₂ was sequestered as immobile mineral phases including dolomite, magnesite, and siderite within the first 10 years. The dissolution trends varied with distance from the injection well, driven by changes in pH and applied reactive surface areas. Spatial variations in cation release (Ca²⁺, Mg²⁺, Fe²⁺) significantly influenced the precipitation of carbonate minerals, leading to up to three orders of magnitude difference in precipitated amounts between simulations employing SSA and ASA. This study demonstrates that fluid accessibility in basalt formations plays a critical role in CO₂ mineralization by influencing mineral dissolution and precipitation dynamics. Moreover, the consideration of reactive surface areas, including SSA and ASA, is crucial for accurately evaluating CO₂ mineralization capacity. These results provide meaningful insights into the utilization of CO₂ mineralization in basalt formations as a reliable and efficient solution for carbon storage.

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MS10 / 396

Extended Analysis of Relative Permeability Curves Using the JBN Method and X-Ray CT Scanning

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The accurate determination of relative permeability is crucial for characterizing multiphase flow in porous media, with direct implications for reservoir simulation and enhanced oil recovery strategies. Traditional methods, such as the Johnson-Bossler-Naumann (JBN) unsteady-state approach, primarily focus on core outlet measurements. This study introduces an extended JBN method that enables the determination of relative permeability curves at specific sections of the core equipped with pressure taps. Additionally, the integration of X-Ray CT scanning provides spatially resolved saturation profiles, significantly enhancing the accuracy and detail of core flooding experiments.

Core flooding experiments were conducted on sandstone samples under controlled conditions of 20°C and 1450 PSI pore pressure. The samples exhibited approximately 21% porosity and 180 mD permeability. Injected water, with a total dissolved solids (TDS) concentration of 36,000 ppm and a CT attenuation value of 231 Hounsfield Units (HU), was doped with 24% NaI to enhance contrast with the oil and rock. EMCA mineral oil served as the non-wetting phase. CT scans were performed at intervals of 0.08 pore volumes (PV) up to the breakthrough point, transitioning to a logarithmic scale thereafter.

The extended JBN method produced relative permeability curves that closely matched those obtained using the standard approach, with differences primarily attributed to error propagation and measurement uncertainties. Additionally, the integration of CT scanning provided detailed saturation distribution profiles, enabling a more comprehensive understanding of fluid behavior within the core. These findings demonstrate the reliability of the extended JBN approach and emphasize the value of incorporating advanced imaging techniques to enhance the spatial precision and accuracy of relative permeability characterization in porous media.

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Doi: 10.1002/2016WR019204; <https://doi.org/10.1007/s11242-019-01369-w>; <https://doi.org/10.1029/2019WR025156>; <https://doi.org/10.1007/s11242-023-01988-4>

Poster / 398

Understanding the influence of fracture network characteristics and fluid density on solute transport in sedimentary fractured rocks

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Complex interactions between geological heterogeneity and fluid properties govern flow and transport in fractured media. These dynamics are critical for applications such as contaminant remediation, enhanced geothermal systems, and geologic carbon sequestration, where density-driven flow can impact transport. Under these conditions, fracture network characteristics significantly control flow paths by inducing preferential flow and contributing non-Fickian transport. Although previous studies have examined the effects of fracture network properties and density-driven flow, we still lack fundamental knowledge about the effects of sedimentary rock features, such as vertical fractures and bedding plane fractures on solute transport.

We developed field-inspired three-dimensional discrete fracture networks (3D DFN) using dfnWorks to systematically investigate how fracture network properties affect solute transport under variable-density flow conditions. The ensembles of DFN models were generated and incorporated fracture and matrix attributes. The domain consists of two 25 m-thick layers representing fractured sedimentary-rock aquifers with four fracture sets: (1) bed parallel parting horizontal fractures (BPP), (2) a vertical injection fracture at the inlet, (3) two sets of stochastic vertical fractures terminated at the layer contacts. PFLOTRAN was used to simulate a pulse injection and transport of tracer into a saturated domain with ambient flow. We examined two structural characteristics: fracture intensity ($P_{32} = 0.01, 0.05, \text{ and } 0.5$) and the presence of BPP, as well as hydrogeological properties, particularly the ratio of vertical to horizontal fracture permeability, under conditions with and without density contrast. Solute breakthrough curves and mass partitioning between fractures and matrix were analyzed to evaluate transport behavior.

The results revealed that BPP significantly influences flow and transport in low- and medium- P_{32} networks but has a minimal effect in high- P_{32} networks. In low and medium P_{32} , BPP induces strong preferential flow, resulting in early solute arrival and multi-modal breakthrough behavior, which is absent without BPP. In addition to BPP, transport is significantly controlled by unique flow paths created by a random distribution of a few vertical fractures, which also cause lower and slower mass recovery. However, a high permeability contrast between vertical fractures and BPP mitigates these unique path effects by limiting solute transport into vertical fractures, promoting a more uniform BPP-dominated flow. In highly fractured networks, the influence of BPP diminishes as enhanced fracture connectivity creates less channelization and more uniform flow throughout the domain, resembling homogeneous media and producing higher and faster mass recovery. However, reducing vertical fracture permeability enhances the influence of BPP and increases flow path heterogeneity, emphasizing the importance of hydrogeological properties in controlling transport. Compared to structural and hydrological factors, the effects of density-driven flow on solute transport were insignificant across all scenarios due to strong dominant fracture flow, especially BPP.

Our findings highlight the role of fracture network characteristics and hydrogeological properties in controlling flow and transport in fractured sedimentary aquifers, where density effects are negligible, as preferential flow paths and permeability contrasts, widely observed in the field, dominate overall flow. However, conclusions may vary slightly under different head gradients that influence fracture flow.

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MS01 / 400

Geochemically induced alteration in geothermal reservoirs and their implications for sustainable energy production**Authors:** Adedapo Awolayo¹; Benjamin Tutolo^{None}; Steve Grasby²; Taylor Smith³¹ *McMaster University*² *Natural Resources Canada*³ *GHD limited***Corresponding Authors:** taylor.smith@ghd.com, awolayoa@mcmaster.ca, steve.grasby@canada.ca, benjamin.tutolo@ucalgary.ca

Geothermal resources constitute a significant portion of the world's low-carbon, renewable energy potential, with about 75% classified as low-temperature (<120 °C). Recent advancements in hot dry rock and engineered geothermal systems have expanded the potential for accessing additional sources of Earth's internal heat, particularly from deep igneous or metamorphic rocks, where heat is effectively trapped by the overlying sedimentary thermal blanket. However, geochemically induced alterations in these highly reactive, low-temperature granitoid resources pose a significant risk to long-term heat production. To assess and potentially mitigate this risk, we conducted a geochemical and mineralogical study to evaluate the geothermal energy potential of Precambrian basement rocks underlying the Western Canada Sedimentary Basin. Through comprehensive characterization, including microscopic imaging, electron microprobe analysis, and Raman spectroscopic mapping of core samples, we evaluated the mineralogical and geochemical changes that have occurred over the basement rocks' history of alteration and how such reactions would have affected the rocks' permeability. Using these interpretations, we parameterized geochemical simulations of water-rock interactions to predict mineral volume changes and their implications for porosity and permeability variations. Our findings reveal that geothermal alteration of the more reactive, unaltered rocks leads to mineral volume changes about 30% greater than those observed in the altered rocks. Utilizing an empirical porosity-permeability relationship, we found that the unaltered basement rocks experienced significant permeability changes. Ultimately, our results suggest that targeting altered, permeable zones within the Precambrian basement rocks could offer more favourable conditions for sustained, multi-decade heat production, making them more viable for geothermal energy exploitation.

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Smith, T., Awolayo, A. N., Grasby, S. E., & Tutolo, B. M. (2024). Investigation of geochemically induced permeability alteration in geothermal reservoirs and its implications for sustainable geothermal energy production. *Applied Geochemistry*, 175, 106193.

MS24 / 401

Accelerating Type 3 Porous Liquid Discovery for Carbon Capture

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Porous liquids (PLs) are an emerging class of carbon capture materials that combine the advantages of solid and liquid state sorbent materials. Type 3 PLs consist of a nanoporous solid sorbent material suspended in an excluded solvent, yielding a liquid with permanent porosity. PL discovery has been largely mediated through iteratively selecting new solid sorbents suspended in ostensibly bulky solvents excluded from the internal porosity of the sorbent material. Recent efforts have sought to systematically identify the impact of solvent properties on PL formation. However, few efforts have evaluated sorbent functional chemistry to discover novel PL compositions. Here we use molecular scale simulations to design ZIF-based PLs for emergent CO₂ capture properties. ZIF-8 was selected as a model nanoporous host due to its stability in multiple solvents, tunability, and intrinsic CO₂ selectivity. Simulated and experimental density was used to evaluate PL formation through prediction of solvent infiltration and resulting porosity. Of the four organic solvents evaluated, the most porous PL composition was composed of ZIF-8 and tetraglyme, followed by acetophenone, glyceryl tributyrates, and then glyceryl triacetate. For these PL systems, CO₂ and N₂ gas sorption isotherms and CO₂/N₂ selectivity were calculated. Additionally, the impact of amine (-NH₂) functionalization of the ZIF-8 surface on solvent infiltration and CO₂/N₂ adsorption was analyzed. By tuning sorbent functional chemistry and solvent identity, the compositional design space for Type 3 PLs was explored. This *in silico* approach results in an accelerated materials discovery timeline and development of chemically informed design rules for PLs with emergent carbon capture properties.

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A Hybrid Conformer Model with 3D Geo-property for Shale Gas Production Prediction: A Case Study.

Authors: Muming Wang¹; Shengnan Chen¹

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This study aims to improve the accuracy and reliability of shale gas production predictions by integrating a Conformer model with 3D reservoir properties, considering well parameters and the geological characteristics surrounding the horizontal wells. A comprehensive analysis of 672 horizontal wells in the Duvernay Formation was conducted to validate the enhanced accuracy and robustness of the proposed approach, introducing new alternatives for predictive modelling in unconventional resource extraction. A novel approach for accurate production prediction was introduced, combining a 3D geo-parameterization technique with a hybrid 3D Conformer module. The 3D Geo-Parameterization method was developed to tokenize the formation properties surrounding the horizontal wells. These geological and well operation features were integrated with a multi-head self-attention-based Conformer model and fused into a unified representation of the horizontal wells' productivity. The integrated multimodality features were subsequently input into three distinct models—LightGBM, XGBoost, and CatBoost—each associated with a specific sampler. Outputs from the three models were finally stacked to predict the well's production. A thorough field study involving 672 horizontal wells in the Duvernay Formation was carried out, demonstrating that the newly developed method achieves an impressive coefficient of determination (R^2) of 0.86 for predicting shale gas production over 12 months. This signifies a remarkable 15.1% average improvement in R^2 and 30.5% mean absolute percentage error (MPAE) decline compared to traditional methods, such as LightGBM and Artificial Neural Network, which relied solely on tabular data and utilized cumulative production figures. This advancement highlights the superiority of the novel 3D geo-parameterization technique and the integration of a 3D Conformer model, demonstrating their effectiveness in unravelling complex geological factors. Incorporating multi-modal inputs and utilizing a hybrid fusion architecture significantly boosts the model's predictive accuracy by reinforcing the relationships between diverse features and shale gas production. Simultaneously, the integration of a self-attention mechanism within the 3D-Conformer architecture plays a crucial role in emphasizing and utilizing the distribution of properties near the wellbore region, thereby enhancing the model's performance. This innovative approach establishes a new benchmark for predictive modelling in unconventional resource extraction. It emphasizes the importance of utilizing unstructured geo-property distribution to enhance the accuracy of production forecasts. This study highlights the transformative potential of combining advanced machine learning architectures with 3D reservoir models for shale gas production prediction. The results advocate for further investigation into hybrid models specifically designed for unconventional resources, emphasizing the benefits of multi-modality parameterization for enhanced performance. Future work will focus on optimizing the model with real-time production data and assessing its adaptability to various geological formations, offering a novel perspective and advancing the application of machine learning in petroleum engineering.

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Upscaling transport in heterogeneous porous media featuring local-scale dispersion: Flow channeling, macro-retardation and prediction

Authors: Scott Hansen¹; Lian Zhou¹

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Many theoretical treatments of transport in heterogeneous Darcy flows consider advection only. When local-scale dispersion is neglected, flux weighting persists over time; mean Lagrangian and Eulerian flow velocity distributions relate simply to each other and to the variance of the underlying hydraulic conductivity field. Local-scale dispersion complicates this relationship, potentially causing initially flux-weighted solute to experience lower-velocity regions as well as Taylor-type macrodispersion due to transverse solute movement between adjacent streamlines. To investigate the interplay of local-scale dispersion with conductivity log-variance, correlation length, and anisotropy, we performed a large-scale Monte Carlo study of flow and advective-dispersive transport in spatially-periodic 2D Darcy flows in high-resolution multivariate Gaussian random conductivity fields. We observed flow channeling at all heterogeneity levels and quantified its extent. We found evidence for substantial effective retardation in the upscaled system associated with increased flow channeling, not attributable to numerical considerations, and for limited Taylor-type macrodispersion, which we may physically explain. A quasi-constant Lagrangian velocity was consistently observed within a short distance of release, allowing usage of a simplified continuous-time random walk (CTRW) model we previously proposed in which the transition time distribution is understood as a temporal mapping of unit time in an equivalent system with no flow heterogeneity. The numerical data set was modeled with such a CTRW and we determined how dimensionless parameters defining the CTRW transition time distributions are predicted by dimensionless heterogeneity statistics. Implications will be discussed.

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Upscaling transport in heterogeneous media featuring local-scale dispersion: Flow channeling, macro-retardation and parameter prediction L Zhou, SK Hansen *Advances in Water Resources* 193, 104830 <https://doi.org/10.1016/j.advwatres.2024.104830>

Poster / 404

A Hybrid Multi-Objective Optimization and Machine Learning Approach for Integrated CCS System Design

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This study introduces a novel hybrid approach combining multi-objective optimization and machine learning to optimize an integrated carbon capture and storage (CCS) system. The method simultaneously addresses both reservoir and facility aspects, solving pipe flow and Darcy's law in porous media based on dynamic nodal analysis. Using CoFlow, an integrated geoenergy system modeling tool developed by CMG Ltd., the study optimizes a CCS system for a potential offshore project in the Republic of Korea. The CCS system features an onshore CO₂ hub terminal, a 175-km subsea pipeline, a 1 km vertical injection well, and a saline aquifer at 1150 m underwater depth. The optimization problem considers four decision variables: CO₂ discharge pressure at the hub terminal, subsea pipeline inner diameter, injection well inner diameter, and CO₂ temperature at the wellhead. Three objectives are targeted: maximizing cumulative CO₂ storage, ensuring safe CO₂ injection pressure, and maximizing the benefit-cost ratio. A multi-objective particle swarm optimization algorithm is combined with CoFlow to derive non-dominated solutions by evaluating approximately 3% of the search space. Machine learning algorithms, including neural networks, random forests, and boosting techniques, are then employed to approximate the entire search space and accurately yield the Pareto-optimal front. The surrogate models' objective function evaluations demonstrate strong alignment with simulation results, validating the effectiveness of the proposed hybrid approach. This methodology offers a valuable tool for field development planning of CCS systems, potentially reducing computational costs while maintaining high accuracy in multi-objective optimization. This study contributes to the growing field of CCS optimization by integrating advanced machine learning techniques with traditional simulation methods, addressing the need for efficient and accurate decision-making tools in complex CCS project planning.

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MS25 / 406

Natural convection facilitates deep mineral leaching and precipitation in a dead-end pore

Authors: Jinil Park¹; Yeonuk Yu¹; Sudong Park¹; Rhokyun Kwak¹; Peter Kang²; Woonghee Lee³; Weon Shik Han⁴

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Mineral dissolution and precipitation significantly impact many geofluid systems, such as carbon mineralization and in-situ leaching. Despite its widespread observation across various fields, the

mechanism to facilitate these reactions has not been proposed yet. In this study, we demonstrated that the natural convection can facilitate mineral dissolution and corresponding precipitation in a dead-end pore for the first time. To investigate this phenomenon, we designed a microfluidic chip featuring a dead-end pore adjacent to a large reservoir, enabling real-time visualization of mineral dissolution, precipitation, and fluid flow. By placing a NaCl crystal in the dead-end pore and AgNO₃ solution in the reservoir, we triggered a reaction where NaCl dissolves, chloride ions react with silver ions, and AgCl precipitates as an insoluble salt. When the pore is positioned at the bottom of the reservoir (aligned with gravity), the reaction ceases rapidly as the precipitate blocks the NaCl crystal. However, when the pore is located at the top, a density gradient forms as NaCl dissolves, inducing natural convection. This convection clears the precipitate, sustaining dissolution and precipitation over time. When the pore is positioned laterally, we observe more complex dynamics: natural convection moves precipitates downward and facilitate dissolution at the upper part, leading to asymmetrical dissolution of the NaCl crystal. Simultaneously, precipitates accumulate from the bottom at the entrance of the dead-end, confining natural convection along the crystal surface. This confinement promotes precipitate growth while establishing a mixing boundary between the dissolved NaCl and the reservoir. A parametric study varying the angle relating the salt dissolution direction to the gravity and AgNO₃ concentrations confirms that the depth and rate of mineral dissolution are proportional to the strength of natural convection. These findings enhance our understanding of gravity-driven mineral dissolution and precipitation dynamics, offering insights with broad implications for scientific and engineering applications requiring deep mineral reactions.

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MS05 / 408

Study of biofilm in porous media in low-temperature geothermal energy context: development and remediation by biocide injection

Author: Alexis Vindret¹

Co-authors: Antoine Margeot¹; Elodie Muller¹; Simon Poirier²; Valentin Guillon¹

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Geothermal power is a promising technology for producing heat and electricity, supporting global decarbonisation efforts. However, this technology can be affected by several operational problems that reduce both profitability and long-term operability. Among them, the development of biofilms in pipes and porosity of reservoir rocks, known as bioclogging, accounts for almost 15% of injectivity problems(1). To counter the growth and spread of biofilms in geothermal installations, remediation methods involving the injection of biocides are commonly employed. However, these treatments are based on tests conducted under non-representative conditions, resulting in unrationalised concentrations and injection protocols. During treatment, only the effectiveness on clogging can be

observed, and the exact bactericidal/bacteriostatic effect is not monitored in situ. This study provides an experimental system and experiments aiming toward a more detailed understanding of this phenomenon under representative conditions.

We elaborated a protocol to study the development of biofilms in porous media and their remediation by the injection of biocides. Flow takes place in anoxic conditions in a cylindrical porous medium with a diameter of 3 cm and a length of 13 cm, constituted of 100 μm Fontainebleau sand, at 30°C and 5 bar. The model bacterial strain, *Shewanella oneidensis* MR-1, was chosen for its ability to form biofilms and its metabolic versatility. In three experiments, sterile supplemented TS growth medium is injected at 5 mL/h in a pore volume of $32,7 \pm 1,6$ mL. For the biocide efficiency assay, benzalkonium chloride (ADBAC) is added to a concentration of 100 ppm, followed by a treatment of HClO- 2000 ppm in water. Biofilm development kinetics were monitored by measuring the differential pressure across the porous medium. Biofilm growth and sloughing were estimated by plating and measuring the OD600 of the effluent. A dissolved CO₂ probe measures in operando bacterial metabolism, and coupled with metabolites concentrations in the effluent (via HPLC) allowed the estimation of the metabolic activity.

For the three experiments, after a stagnation phase of 24-72 h, a biofilm develops and stabilizes over 96-192 h of injection. Bioclogging was variable, with differential pressure increases of 200-1500 mbar, a bacterial population in the effluent ranging from 108-1010 UFC/mL, along with an increase in OD600 between 0.04 and 1. It is also linked with the consumption of ~95% of lactate/fumarate, and production of succinate/acetate up to ~95% of theoretical stoichiometry. When treated with ADBAC 100 ppm, metabolic activity is reduced by ~95%, bacterial concentration in the effluent is reduced by 100 to 1000-fold over 143 to 190 h and OD600 reaches zero after 70-183 h. However, permeability is not regenerated and remained between 140 and 1100 mbar. HClO- 2000 ppm treatment restored ΔP to 14-17 mbar in 67 hours.

Biofilm in a porous medium was formed and both physical and biochemical characteristics were followed. While ADBAC significantly reduced bacterial viability, bioclogging required a strong oxidising solutions to be eliminated. Future experiments will study the effectiveness of another widely used biocide in geothermal energy, glutaraldehyde, and compare it to ADBAC for a more responsible use in industrial conditions.

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MS07 / 410

A Multiscale Approach to Simulate Multiphase Non-Isothermal Flow in Deformable Porous Materials

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Feedbacks between multiphase fluid flow and solid deformation are crucial for advancing many geotechnical applications. These feedbacks remain incompletely understood and challenging to represent, particularly in complex porous media with pores of varying sizes. Traditional hydraulic-mechanical coupled models often struggle to accurately represent hybrid systems that include both solid-free regions and porous media. The Darcy-Brinkman-Biot (DBB) framework has been demonstrated to effectively capture capillary, viscous, inertial, interfacial, and gravitational forces at both pore and Darcy scales. The solver converges to the solution of the two-phase Navier-Stokes equations at the pore scale, while it tends asymptotically toward the solution of the two-phase Darcy equations at the continuum scale.

In this study, we extend the DBB framework, originally based on isothermal conditions, to model non-isothermal problems. By incorporating a new energy conservation equation, we develop a solver called `hybridBiotThermalInterFoam`, implemented in the Computational Fluid Dynamics (CFD) software OpenFOAM. This model accounts for the temperature dependence of fluid viscosity, fluid density, surface tension, and permeability. We validate the new solver by comparing its results with analytical solutions for heat transfer in systems with two fluids and against other OpenFOAM heat transfer solvers, such as `chtMultiRegionFoam`. The new solver shows excellent agreement with both the simplified analytical solutions and numerical predictions.

To further demonstrate the versatility of the solver, we apply it to more complex cases, including an enhanced oil recovery (EOR) scenario where high-temperature water and supercritical CO₂ are injected into an oil-saturated porous medium to study fingering phenomena under dynamic mobility conditions. Additionally, we simulate a hybrid-scale case where fluids such as water and glycerin are injected into a soft clay-like material in the presence of induced fractures. The results show that the new solver effectively predicts heat transfer in multiphase fluids and deformable solids exposed to strong thermal fluxes, with potential applications in a wide range of coupled thermal-hydraulic-mechanical-chemical problems. To our knowledge, this is the first model capable of representing multiphase, non-isothermal fluid flow in deformable porous media within a hybrid system.

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MS02 / 411

Development of an Integrated Biofilm NMR Microplastic Sensor for Agricultural Water Monitoring

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A laboratory investigation aimed at understanding the interaction between model environmental biofilms and water quality contaminants such as metals and microplastics is developed. Microbial biofilms can adsorb and retain water-born contaminants in their matrix of extracellular biopolymers, which form a hydrogel called EPS, and therefore have potential to capture evidence of transient contamination events in surface and irrigation waters. Metals, like copper and lead, as well as microplastics are contaminants of emerging concern and pose risks to the safety of the food supply when they appear in irrigation water. Each of these contaminants is also visible using nuclear magnetic resonance (NMR) relaxometry. Metals in water cause changes in NMR signal relaxation; microplastics have different signal relaxation properties than water and interact with the water molecules in biopolymer crosslinking, which are detectable by relaxometry and magnetic resonance imaging (MRI) experiments. Laboratory experiments using two model biofilms –sodium alginate beads and a multispecies biofilm, aerobic granular sludge, to assess sorption and evolution of target contaminants are undertaken. The novel data obtained can be integrated with low field NMR sensors in the field to aid in the detection of diverse contaminants in water supply and irrigation systems, potentially including transient contamination events.

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Poster / 412

About approaches to large-scale simulation of CO₂ plume characteristics at realistic conditions

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The fundamental importance of CO₂ trapping mechanisms during geological storage in deep saline aquifers (DSA) remains indisputable and requires adequate means for adequate description and successful application. During last decades tremendous efforts have been made in many research areas to provide experimental, theoretical, simulation and pilot tests data at diverse conditions and multiple description scales [1,2], see also the references in [1]. One of the essential lessons learned during this period was the recognition of many issues where the huge power inherited from the conventional reservoir simulation is insufficient from the viewpoint of geological storage applications. It's enough to mention that this is true, for instance, for completely different characteristic time and space scales of typical storage cases, especially in view of upcoming stage of the storage sites clustering [3]. Since the beginning of pioneering CO₂ storage pilot, the reservoir-scale simulation has contributed much to general understanding of the process dynamics and to assessment of the storage data. Nevertheless, up to now the dedicated reservoir simulators seem hampered, especially in direct realistic simulation of storage cases which comprises evaluation of several principal trapping mechanisms, cf. eg. [4].

Our current work is aimed at development and testing of approaches to modelling capable to provide simulation results for realistic storage cases on the base of enhanced computational performance [5].

The indispensable elements of this work include the definition of relevant description for and quantification of CO₂-in-brine dissolution dynamics. Recently convective dissolution and its dynamics were found to be influential factors in the CO₂-plume evolution during injection and post-injection periods of the storage. Moreover, they can impact the key indicators of geological storage like its efficiency and spatial limits of the CO₂ plume.

Taking advantage of our recent experience involving the studies of dissolution for typical conditions of Utsira and also for one of typical sites called in literature “natural analogues for CO₂ storage” [6], the extension of numerical analysis towards generalization of dissolution dynamics for anisotropic and heterogeneous DSA has been carried out. Currently, the dynamic dissolution process in heterogeneous porous media represent a paramount challenge of density-driven flow dynamics [7]. The methodological aspects of (1) enhanced performance models and their development and (2) theoretical approach to quantification of convective dissolution in a heterogeneous aquifer, are discussed in some details. Also, the discussion together with corresponding illustrations are provided on the feasibility of reported approach to simulation of CO₂ plume dynamics and possible directions of the work extension in nearest future.

Analysis of conditions when dynamic CO₂ dissolution in an aquifer brine may impact the plume parameters and shape during post-injection can play a role in the adaptation of design and monitoring strategy for geological carbon storage sites.

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MS16 / 414

Evaporation and absorption of surfactant-laden droplets on unsaturated porous media

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Understanding the evaporation and absorption of surfactant-laden droplets on porous media is challenging and important for many industrial applications, such as inkjet printing. Fast penetration of the droplets is desirable to minimize the time droplets remain on the paper, thereby preventing the coalescence of droplets, which is an undesirable outcome in inkjet printing. The addition of surfactants can alter the surface energy of the liquid-gas interface in the paper, possibly accelerating the penetration rate of droplets(1,2). Surfactants can also suppress the coffee-ring effects in the droplet, resulting in a more uniform deposition ink pattern, further improving the inkjet printing quality(3,4). Therefore, understanding the imbibition of surfactant-laden ink into paper is critical for optimizing inkjet printing. The complexity and visualization difficulty of porous media, and the interaction between fluid dynamics and surfactants make this a challenging problem.

The evaporation of surfactant-laden droplets on a fibrous thin paper sheet is a 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-adsorption model is employed, including adsorption at both the liquid-air and liquid-solid interfaces.

We first simulate one-dimensional (1D) absorption of surfactant-laden ink into unsaturated porous media to investigate the influence of parameters, such as porosity, Peclet number (Pe), Damköhler number (Da), and maximum adsorbed surfactant concentration, on the absorption dynamics. This analysis also allows us to study the similarities and differences compared to saturated flow models. Then we extend our study to two-dimensional (2D) problems assuming axial symmetry in cylindrical coordinates, incorporating droplet dynamics and liquid-air interface adsorption in unsaturated regions. This extension contribute to advancing our understanding of complex dynamics involved in surfactant-laden droplet absorption in porous media.

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Wettability and Interfacial Behavior of CO₂-Brine-Oil Systems in Nanopores: Nanoscale Analysis and Modification of Classical Equations

Authors: Kaiwen Tang¹; Wendong Wang¹; Chengwei Wang¹; Shiyuan Zhan²; Jilong Xu³; Yuliang Su¹; Lei Li¹; Yongmao Hao¹

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In the context of the widespread use of CO₂-enhanced oil recovery, it is crucial to understand the mechanism of the synergistic effect of ions and CO₂ on the wettability of oil and water phases. However, due to the confinement effect at the nanoscale, it is difficult for traditional theories to accurately characterize the structure and interfacial properties of nano-droplets in inorganic pores of shales. The objectives of this study are as follows: a) to reveal the adsorption mechanism of brine liquid films in kaolinite pores and the mechanism of changes in oil-phase wettability; b) to accurately trace the position of the oil-brine interface, and introduce a modified Edwards-Wilkinson equation that considers linear tension, surface tension and molecular interactions; c) to modify Young's equation to apply to nanoscale systems by introducing interfacial fluctuations and linear tension effects.

We constructed a molecular dynamics model of a system of brine-multicomponent hydrocarbons (methane, n-octane, and tetradecane) containing CO₂ in the interstitial spaces of kaolinite, gibbsite surfaces, and siloxane faces. Through simulation, we statistically analyzed the density distribution of each component, the interfacial fluctuation characteristics, and the intermolecular interactions. The interface detection algorithm was improved, and the space-time correlation function of the liquid-liquid interface position and interfacial tension was analyzed. A method for characterizing interfacial wettability based on the potential of interaction was proposed. Based on these analyses, the Edwards-Wilkinson equation and Young's equation were modified to more accurately describe interfacial behavior and wettability changes at the nanoscale.

On the kaolinite-gibbsite surface, strong water-molecule-surface interactions and an ordered ionic structure maintain a low interfacial energy. CO₂ slightly increases the interfacial energy, but overall maintains hydrophilicity and suppresses interfacial fluctuations. In contrast, on the relatively hydrophobic kaolinite-siloxane surface, the adsorption of CO₂ significantly reduces the interfacial energy, enhances hydrophobicity, and increases interfacial fluctuations. In light of these observations, we have modified the Edwards-Wilkinson equation and the Young equation to account for the effects of line tension, surface tension, and intermolecular interactions. Our modifications take into account the effect of interfacial curvature on the local potential energy distribution and the regulatory effect of CO₂ concentration on interfacial energy. We have also introduced terms related to CO₂ concentration and ionic strength into the Edwards-Wilkinson equation to more accurately describe interfacial wetting behavior.

Improved interface detection and time-space correlation analysis reveal the strong influence of CO₂ concentration on the wettability of the oil phase. The modified Edwards-Wilkinson and Young equation, which incorporates line tension and molecular interactions, accurately describes interfacial behavior and wettability changes at the nanoscale.

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Poster / 416

Contaminant Transport Modelling using FEFLOW in Eastern Coastal State of India

Author: Kamalakanta Sahu¹

Co-authors: Sumedha Chakma¹; Yellamelli Ramji Satyaji Rao²

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Groundwater, while abundant, remains highly susceptible to contamination from industrial effluents, improper waste disposal, and excessive agricultural fertilizer use. In recent years, the improper application of nitrogen-based fertilizers has significantly contributed to nitrate contamination in the groundwater systems of eastern coastal India. This study focuses on two vulnerable regions in Odisha to analyse contaminant transport mechanisms and aquifer dynamics. Utilizing input parameters, shapefiles, and borewell datasets, we employed FEFLOW software to simulate and visualize the three-dimensional movement of nitrate contaminants over a 50-year period. The results indicate a notably faster contaminant migration in Sundargarh compared to Sambalpur, primarily due to differences in aquifer disposition and fertilizer application practices. This research provides critical insights for optimizing fertilizer management strategies and implementing sustainable water resource management practices to ensure safe, nitrate-free drinking water in the region.

Keywords: Modelling, transport, nitrate, contamination, and FEFLOW.

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Assessing Hysteresis and Heterogeneity for Optimized Hydrogen Storage in Aquifers

Author: Abdolali Mosallanezhad¹

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In line with global climate targets, the transition to net zero carbon emissions by 2050 underscores the critical need for adopting low-carbon energy solutions. Among these, hydrogen has emerged as a cornerstone for decarbonisation efforts. However, the scalability of hydrogen storage systems, particularly in geological formations, poses significant challenges. This research examines underground hydrogen storage in saline aquifers, focusing on the effects of reservoir heterogeneity, hysteresis, and injection/production dynamics. Simulations were performed to analyse the effects of hysteresis, injection/production rates, and permeability on storage performance.

Two heterogeneous systems featured the same omni-directional spatial continuity and average absolute permeability of 100 and 500 mD were simulated in a 2D Cartesian system (Figure 1). Injection rates were restricted by the fracturing pressure (20000 kPa), while production rates were limited to maintain a minimum well bottom-hole pressure of 5000 kPa. A constant pressure boundary (infinite-acting aquifer) served as a spill point, providing sufficient capacity for gas movement and ensuring steady flow rates during injection and production cycles. An observation well was placed at the model's centre to monitor hydrogen saturation change. As soon as hydrogen reaches this point, the injection stops until the next cycle begins to prevent hydrogen loss.

The experimental relative permeability data for primary drainage (PD) and secondary imbibition (SI) reported by Lysy et al. (2022) were utilised to develop the relative permeability and capillary pressure curves, including hysteresis behaviour. The residual gas saturation was set at 0.36, consistent with the experimental data (Hashemi et al. 2021, Rezaei et al. 2022), while the critical gas saturation values were modified based on studies involving similar core properties. These adjustments ensured that the curves represent hydrogen and water flow dynamics in porous media, as reflected in

Figure 2.

Performing a series of simulations determined that the optimal injection and production rates are 3.5 m³/day and 14.1 m³/day, respectively, for models with average absolute permeabilities of 100 mD and 500 mD. These rates effectively maintain pressure fluctuations within the target range. Additionally, the selected rates ensure that the gas front does not reach the observation well, preventing interruptions to the injection cycles based on the predefined conditions.

For the 100 mD model, the recovery factor increases from 57.7% to 82.4%, while for the 500 mD model, it rises from 52.4% to 74.1%. This improvement reflects reduced gas trapping and stabilised flow dynamics. The higher recovery in the 100 mD model is due to more uniform gas distribution and less bypassing, while the 500 mD model shows inefficiencies from reservoir heterogeneity and higher gas mobility.

In summary, this work shows that hysteresis impacts capacity and recovery, heterogeneity in the high permeable reservoir causes gas fingering and reduces efficiency, and selecting flow rates requires balancing hydrogen recovery and reservoir pressure.

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MS02 / 419

Exploring Water Transport and Aging Mechanisms in Bio-Based Porous Materials through NMR Relaxometry

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Aluminosilicate-based materials, such as geopolymers, have attracted significant attention due to their diverse industrial applications in catalysis, adsorption, and wastewater treatment. Among these materials, aluminosilicate hydrogels, precursors to zeolites, show great promise for advancing sustainable materials. These hydrogels are capable of enhancing soil stabilization and reducing environmental impacts. Characterized as colloidal fractals, they undergo temporal transformations, including syneresis (water expulsion) and crystallization into zeolites, particularly under drying conditions [1]. Despite their potential, the complex mechanisms driving these changes are not yet fully understood, highlighting the need for detailed studies to unlock their full capabilities. A comprehensive understanding and precise monitoring of these dynamic processes are essential for optimizing these materials for eco-friendly applications, in line with the principles of green chemistry aimed at minimizing the environmental footprint of industrial processes.

In this study, to explore these processes, we use Nuclear Magnetic Resonance (NMR) relaxometry, an advanced and non-destructive technique, to monitor water dynamics within these gels with high temporal resolution. We combine global measurements using T2 relaxometry with localized spatial assessments through 1D profiles. This dual approach allows us to capture both large-scale changes in the water status of the material and detailed spatial variations, especially those associated with significant deformation during drying. We also study the aging processes of these gels to investigate how water retention and structural stability evolve over time. Our results demonstrate how environmental conditions, such as drying and temperature fluctuations, influence the porosity and stability of these materials, demonstrating NMR potential to track gel phase evolution under varying conditions.

This approach provides valuable insights into the water dynamics of aluminosilicate gels, enhancing our understanding of their behavior in sustainable applications. By integrating generalized NMR dynamic relaxometry [2], we applied this methodology to various aluminosilicate formulations with different NaOH concentrations, revealing a power-law behavior in the water dynamics. This result underscores the complex relationship between gel structure and water mobility during the drying process. To further investigate this phenomenon, we conducted simulations to explore the underlying mechanisms driving the power-law behavior and its impact on the material properties.

In the future, we plan to extend this methodology to study other bio-based porous materials, from wood to living plants, which play key roles in sustainable construction. By comparing the water dynamics across these materials, we aim to contribute to the advancement of bio-based materials for applications in construction and agriculture sectors.

Keywords: Aluminosilicate hydrogels, NMR relaxometry, water dynamics, sustainable construction, green chemistry, agriculture, zeolites, bio-based materials, soil stabilization, porous media.

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420

Generalized network modelling of pore-scale displacement in multiscale carbonates

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The Generalized Network Model (GNM) enhances pore-scale flow predictions by realistically representing pore spaces and fluid interfaces, including expanding-contracting throat geometries, with corner conductivities determined through direct numerical simulations (Raeini et al., 2017; 2018). However, micro-computed tomography (μ CT) resolution limits the smallest pores represented in the extracted network. This poses challenges for modelling multiphase flow in complex, multiscale carbonates with intricate connectivity. To address resolution limits, we developed a multiscale GNM that leverages differential imaging of dry and high-contrast saturated sample to visualize and quantify interconnected but unresolved porosity in three dimensions. Microporous voxels in the differential porosity map are grouped based on their proximity to nearby resolved pores using an automated dilation process (Foroughi et al., 2024). This process forms additional throat types, referred to as microlinks, which connect in parallel or series with the macro network, facilitating percolation through microporosity independent of macro-throats. We treat microlinks as a continuous Darcy-type porous medium and, thus, employ classical empirical relationships to describe flow within them. In addition, the single scale GNM—previously validated for homogeneous rocks—is enhanced to better assign resolved connectivity within complex carbonates through a modified corner connectivity assessment. The multiscale GNM was tested on three carbonate samples—two Ketton limestones and one reservoir carbonate—exhibiting increasing heterogeneity. The model was calibrated with mercury intrusion capillary pressure and differential imaging-based porous plate drainage data. Model predictions for drainage behaviour align within the uncertainty range of capillary pressure experimental measurements, revealing the distinct roles of macropores, unresolved intermediate-sized pores, and micropores during an invasion-percolation process. This approach offers a robust and computationally efficient method for incorporating sub-resolution porosity, enabling a detailed representation and more accurate predictions of natural and engineered multiscale porous systems.

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MS01 / 421**Redox reactions in near-wellbore tight rocks during gas storage****Author:** Qingyun Li¹¹ *Stony Brook University***Corresponding Author:** qingyun.li@stonybrook.edu

Carbon sequestration and hydrogen storage at large scales require suitable subsurface formations, with shale playing critical roles in both scenarios. In conventional reservoirs, shale acts as a caprock, preventing the upward migration of injected gases. In unconventional reservoirs, hydraulically stimulated shale contributes to storage by providing fractures, cracks, and pore spaces.

The injection of gas from the surface induces shifts in chemical equilibria due to rock-water-gas interactions. While mineral dissolution and precipitation have been extensively studied for their effects on pore structure and hydraulic conductivity, redox reactions remain less explored. These reactions, however, are crucial due to their implications for nutrient cycling, microbial activity, and heavy metal mobilization.

This presentation will cover my recent studies that involve iron and sulfur redox reactions in shale after either carbon dioxide or hydrogen injection. These experiments were designed to simulate near-wellbore conditions where shale is exposed to relatively fresh injected gas in the presence of formation brine, with some systems also incorporating wellbore cement. Our findings indicate that in carbon sequestration systems, the injected gas shifted the environment toward oxidative, whereas in hydrogen storage systems, it became chemically reductive. The extent of these redox reactions was influenced by complex factors, including the injection sequence and the presence of wellbore cement.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

Anna Lisa Herring

MS03 / 422

Impact of Stress and Fracture Orientation on Fluid Mixing at Fracture Intersections

Authors: Jingxuan Deng^{None}; Laura Pyrak-Nolte¹; Peter Kang²

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Fractures and fracture networks are critical pathways for subsurface flow and reactive transport in rock. In particular, fracture intersections, where fluids with different properties mix and react, serve as biogeochemical reaction hotspots. Recent studies have highlighted the importance of intersection geometry in influencing mixing dynamics. Although geologic fractures are subjected to geological stress, the impact of stress-induced geometric changes on mixing at intersections remains unexplored. In this study, we combine laboratory experiments and 3D pore-scale numerical simulations to investigate how stress-induced changes of intersection geometry affect mixing at fracture intersections and discuss the implications for upscaled modeling of mixing at fracture intersections.

For the laboratory experiments, four 3D-printed prismatic blocks were used to create a fracture intersection between two orthogonal fractures. The behavior of the orthogonal fracture intersections was examined for two orientations relative to the applied load. An “×” intersection occurs when the direction of gravity is at a 45-degree angle with respect to the fracture planes, while a “+” intersection occurs when the direction of gravity is parallel to the vertical fracture. The samples were weakly laterally confined while subjected to a normal load that was oriented along the direction of gravity. 3D X-ray tomographic reconstructions of the geometry of the intersecting fractures were used to generate numerical meshes for flow and transport simulations. The numerical simulations were conducted by solving the steady-state, incompressible Navier-Stokes equations for the flow and the advection-diffusion equation for solute transport and mixing.

Our results reveal that both the stress magnitude and the orientation of fractures relative to the direction of maximum principal stress exert dominant control over deformation, which in turn controls fluid flow and mixing. In the “+” intersection, as the load increases, the horizontal fracture mainly closes while the vertical fracture remains unaffected. The closure of the horizontal fracture increases flow and solute mass flux toward the vertical fracture. In the “×” intersection, an increase in load induces shear dilation, causing one fracture to open while the other closes. Additionally, contact areas form near the region where the two fractures intersect due to shear dilation and expand as the load increases. This shear-induced contact areas transform the intersection from an “×” shape into two “v”-shaped fractures connected by critical links, referred to as pinch points. Shear-induced dilation opens one fracture, leading to increased flow and solute mass toward the opening fracture. However, continued loading reduces void the number and the volume of pinch points, limiting further flow increases despite the growing aperture difference. Current network-scale modeling does not account for the effects of stress on mixing at intersections, potentially leading to overpredictions of mixing. To address this, we propose a simplified mixing model that captures the key processes. This study suggests that the stress state and fracture intersection orientation are the key factors controlling mixing and transport in fracture networks.

ACKNOWLEDGEMENTS

We acknowledge support from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Geosciences Research Program (Award Number DE-SC0001048) for the laboratory work.

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MS15 / 424

Identifying Aquifer Recharge Signatures Using Unsupervised Machine Learning: A Case Study of the Pajarito Plateau, NM

Authors: Bulbul Ahmmed¹; Noah Hobbs¹

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The Pajarito Plateau shallow aquifer is a crucial resource for Los Alamos town, New Mexico. Changes of the shallow aquifer level could have a large environmental impact where water scarcity can concentrate pollutants and negatively affect the local ecosystem. The shallow aquifer recharge is poorly understood because of the area's complex geology, and is extremely sensitive to climate change. Traditionally, the recharge (source) amount is determined with a parameter estimation study using hydrogeological models. These models require the input of climate data (temperature, precipitation estimates), topographic data, soil and vegetation data, geologic data (rock formation permeabilities, faults, etc.), and huge computational resources. To circumvent these limitations we investigate the use of non-negative matrix factorization with customized k-means clustering (NMFk), an unsupervised machine learning model, to identify climate source signatures and their effect on groundwater fluctuations. NMFk only requires temporal hydraulic head data from wells to obtain a set of potential signatures. Therefore, it has the advantage of relatively brief data acquisition and processing times, as well as short model run-times. The resulting source signatures represent the effect of precipitation on the aquifer levels; we match these signature profile(s) to observed climate signatures (i.e., average precipitation, snowmelt) to understand the relationships between the competing water sources. The machine learning model results show the influence of each signature at each well. Moreover, using signature intensities for each well, we found that snowmelt on the Pajarito Plateau and a combination of snowmelt and storm runoff from the higher elevation areas adjacent to the plateau are the main drivers for the shallow aquifer recharge. Moving forward, the NMFk model results will be combined with climate models to construct more accurate hydrogeologic models. These models will help understand how the aquifer could be affected by future climate change.

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Poster / 425

Dual Energy X-Ray CT for Improving the Characterization of Clay-Rich Sandstones

Author: Cinar Turhan¹

Co-authors: Jonatas Castro Einsiedler²; Masa Prodanovic¹; Richard Alan Ketcham¹; Rodolfo Araujo Victor²

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Dual-energy computed tomography (DECT), a non-destructive characterization method of geological samples, has been used for estimating the effective atomic number (Z_{eff}), and the density (ρ) of the components of a sample. These estimates require calibration using three materials with known intensities as well as air –typically surrounding the sample –within the scan range, resulting in four reference points at two different X-ray energies. This type of setup is not standard practice, but we argue that it should be.

CT data always contains noise. Incorporating a Monte Carlo (MC) approach into this method quantifies the uncertainty caused by the noisy nature of CT scans, and allows for finding a solution where noise would prevent finding an exact solution. A study by Victor et al. (2017) showed that this method can be used in carbonate samples to improve the estimation of petrophysical properties; however, its application remains untested in clay-bearing sandstones and other rock types. In this study, we validate the application of MC-based inversion of Z_{eff} and ρ in clay-rich sandstones and assess its effectiveness. We focus in particular on improving the saturation estimates, which are often unreliable for clay-rich materials, as well as distinguishing clay types.

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Poster / 427

Impact of Synthetic Laminar and Vugular Heterogeneities on USS Core Flooding Outputs

Author: Caroline Henrique Dias¹

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SCAL (Special Core Analysis) tests are essential for determining the properties of heterogeneous porous media under multiphase internal flow, including capillary pressure, relative permeability, and wettability. These tests are pivotal for predicting reservoir performance. Among them, the USS (Unsteady-State) core flooding test is particularly noteworthy. In this test, an oil-saturated rock sample, initially at irreducible water saturation, is subjected to a controlled water flow at one end. This process displaces oil, which is produced at the opposite end until breakthrough occurs, after which both oil and water are produced. The test enables the evaluation of permeability and saturation under conditions that mimic a petroleum reservoir environment. The significance of this experiment is heightened when the goal is to investigate the properties of highly heterogeneous rocks characterized by elongated and irregular volumetric discontinuities, such as laminar and/or vugular heterogeneities. These structures significantly influence the dynamics of water saturation within the porous medium. However, boundary experimental data, such as cumulative oil production and pressure differential, often fail to capture these changes, making distinguishing between strongly heterogeneous structures challenging. In this context, the present study examines the impact of synthetic laminar and vugular heterogeneities on the experimental outcomes of the USS core flooding test, intending to determine whether these features can be characterized in a transient test. Three primary experimental outputs were analyzed: the pressure differential between the two ends of the rock, cumulative oil production, and saturation profiles along the core. The investigation focused on parameters such as the thickness, quantity, and permeability ratio of laminations relative to the core in laminar heterogeneity, as well as the quantity, size, and distribution of vugs in vugular heterogeneity. Three-dimensional simulations were conducted using the CMG software in a computational environment. The experimental design revealed that certain parameters exert a significantly greater influence than others and that some experimental outputs cannot differentiate the medium's heterogeneity. This limitation renders these outputs potentially ineffective for subsequent uncertainty quantification in the analysis of these porous media of interest.

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Poster / 428

Sensitivity Analysis and Experimental Design on Relative Permeability and Capillary Pressure Parameters in Experimental USS Core Flooding Data

Author: Gianfranco de Mello Stieven¹

Co-authors: Filipe Oliveira da Silva ¹; Caroline Henrique Dias ¹; Antonio Emanuel Marques dos Santos ¹; Paulo Couto ¹

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The computational simulation of petroleum reservoirs is crucial for understanding the dynamics of multiphase flow in geological formations, enabling the development of advanced models and accurate predictions. These simulations rely heavily on parametric constitutive relationships to represent fundamental reservoir engineering properties, such as relative permeability (k_{rel}) and capillary pressure (p_c). These properties are indispensable for modeling multiphase flow on a continuum scale in heterogeneous porous media. Reliable oil production estimates, in turn, require the quantification of uncertainties associated with system property parameters. This quantification establishes upper and lower bounds for the economic feasibility of reservoir development. However, most models in the literature depend on numerous empirical parameters that must be determined. Despite their complexity, these parameters often lack a direct connection to the underlying physics of the problem. Furthermore, preliminary sensitivity and linear dependence analyses of these parameters are essential but are frequently overlooked, especially in unsteady-state (USS) core flooding experiments. Such analyses help determine whether a parameter can be effectively estimated before proceeding to uncertainty quantification. In this context, the present study investigates the sensitivity coefficients and experimental design of relative permeability and capillary pressure parameters, both parameterized using the LET model, in single-step USS core flooding experiments conducted on real rock samples. In these experiments, a core plug saturated with oil is subjected to axial water injection at one end, leading to oil production (and, after breakthrough, water production) at the opposite end. The experimental data include the pressure difference between the water inlet and the oil (and water) outlet, as well as the cumulative oil volume produced. Computational simulations were conducted using the open-source Core2RelPerm code to model the flow, in combination with the heuristic optimization method Particle Swarm Optimization (PSO). This approach was employed to optimize the relative permeability and capillary pressure parameters, using the two experimental outputs as boundary conditions. The optimization process enabled the reconstruction of the water saturation profile along the core—data that are not directly accessible from the experiments. This reconstruction provided valuable insights into the dynamics of water saturation development in different cores. Subsequently, sensitivity coefficients for the experimental design of all investigated parameters were determined across various rock samples, using the experimental outputs and the reconstructed water saturation profiles from the optimization. The results indicate that only a small subset of the studied parameters exhibit significant sensitivity, highlighting the potential overparameterization of the employed parametric model. Additionally, it was observed that certain experimental responses are more critical than others, based on the magnitude of parameter sensitivity associated with those responses. The experimental design also suggests the possibility of conducting these experiments in a shorter time frame, thereby reducing their execution costs.

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MS09 / 429

Capillary Pressure-Saturation relation derived from the Pore Mor-

phology Method

Authors: Fernando Alonso Marroquin¹; Martin Andersson¹

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A computational-efficient method to calculate capillary pressure-saturation relations of immiscible, multiphase flow on two-dimensional pore morphologies is presented here. The method is an extension of the Pore Morphology Method that includes wetting angle and trapped mechanism of the displaced fluid. After validating the method with micro-chip fluid injection experiments, the method is used to relate pore morphology to capillary pressure-saturation relation using square-lattice pore morphologies. Because the method uses only morphological binary operations, it is more efficient than well-established high-resolution voxel dynamics methods such as Lattice Boltzmann Methods and Level-set computational fluid dynamics. Apart from pore morphology, only the material parameters related to contact angle (wettability) and interfacial tension, are required to connect the pore-saturation relation and pore throat distribution. We investigate the effect on interfacial tension, wettability, and sample size and pore throat distribution on entry pressure and residual saturation.

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MS11 / 433

PORE-SCALE VISUALIZATION AND ANALYSIS OF MULTIPHASE FLOW IN FRACTURED POROUS MEDIA

Authors: Vivian M. de Sousa¹; Brenda Maria De Castro Costa¹

Co-authors: Jorge Avendaño¹; André Luiz Martins Compan²; Marcio Carvalho¹

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Naturally fractured reservoirs contribute approximately 25–30% of global oil production. The presence of fractures, vugs, and interconnected channels introduces complexities in fluid flow within

rocks, either by creating preferential pathways or acting as barriers (1). This study seeks to advance the understanding of fluid behavior in fractured rocks and their associated characteristics. To achieve this, we use a lab-made reservoir-on-a-chip (RoC) devices to investigate and visualize pore-scale fluid dynamics in fractured porous media, enabling the correlation of macroscopic properties with microscopic two-phase flow behavior.

The micromodels used in this work feature a porous matrix, made of a random arrangement of straight and constricted microchannels with different width, embedded with different fracture geometries (2). The experimental setup incorporates an inverted microscope and a high-speed camera for real-time visualization of phase distribution and image acquisition. Pressure gradients are monitored using transducers integrated into the microfluidic system.

Simultaneous water and oil injection experiments at different water fractional flow rates were performed to obtain relative permeability curves and phase distribution for both fractured and non-fractured porous media. The results reveal that the two-phase flow through the fracture evolves from a slug to stratified flow regime as the non-wetting aqueous phase fractional flow rate increases. The presence of the fracture alters significantly the phase distribution within the pore space and the flow dynamics. The changes in relative permeability and capillary pressure curves associated with the presence of the fracture is analyzed for different fracture geometry.

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MS02 / 434

Quantifying water flow across and hydraulic conductivity of the rhizosphere in coarse-textured soils using high-resolution X-ray CT

Author: Patrick Duddek¹

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Plants are major drivers of terrestrial water fluxes, transpiring 40% of the global terrestrial precipitation. This vast amount of water inevitably flows through the rhizosphere, the thin soil layer

surrounding roots. This interface is, therefore, of great relevance for the hydrological cycle. Especially when considering coarse-textured soils such as sandy soils, existing soil-plant models significantly overestimate the water flow in the rhizosphere, consequently overestimating transpiration in drying soils. This discrepancy reflects the challenges in estimating the hydraulic properties of the rhizosphere, particularly in sandy soils where most of the losses in water potential directly occur in the first millimeter near the root-soil interface. At this small scale (< 1 mm), the existing definition of hydraulic conductivity falls short. Additionally, the contact area between root and soil water changes substantially as the soil dries. Currently, we lack a quantitative description to accurately estimate the water flow across the heterogeneous and dynamic rhizosphere.

By means of high-resolution synchrotron radiation-based X-ray computer tomography (act. pixel size $0.65 \mu\text{m}$), we study the rhizosphere of 8-day-old maize (*Zea Mays* L.) roots grown in sandy soil (sample diameter 8 mm). Novel AI-based image segmentation and analysis techniques enable us to quantify the connectivity of the liquid phase across the rhizosphere at varying soil water potentials. The three-dimensional segmented images are used to simulate the flow of water and air in the rhizosphere. The simulations enable quantitative estimation of the effective hydraulic conductivity of the rhizosphere.

Our analysis shows an important loss in contact area between roots and soil water at relatively high soil matric potentials and decline in the connectivity of the liquid phase across the rhizosphere. This results in a restriction of water flow paths from the bulk soil to the roots and a reduction in hydraulic conductivity. To incorporate this observed behaviour of the rhizosphere hydraulic conductivity in upscaled models, we developed a scheme that allows us to estimate an effective rhizosphere hydraulic conductivity. This parameter is crucial, particularly in sandy soils, for accurately including the rhizosphere in upscaled root water uptake models.

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435

Determination of multi-phase flow characteristics of micro-porous heterogeneity in multi-scale porous media using deep learning

Author: Muhammad Ali¹

Co-authors: Dmytro Petrovskyy ; Hannah Menke¹; Julien Maes¹; Kamaljit Singh¹

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Subsurface porous rocks hold significant storage potential for both carbon sequestration and hydrogen storage. To achieve maximum storage capacity and counter possible operational challenges, the geo-physical characteristics of the sub-surface rock needs to be analysed thoroughly, which is extensively carried out using CT-images. However, within the CT-images, there are unresolved phases

which are not classified as solid grain or pores, but rather as porous heterogeneities. These unresolved phases present a challenge in accurately predicting the geo-physical characteristics of the rocks.

In this work, we present an approach to characterise the micro-porous heterogeneities using a multi-modal deep learning predictive model. The task is setup as an inverse problem where the model is trained to predict the input parameters required for multi-scale flow simulations by providing the results computed from the simulation. Here, we have trained the model to predict the porosity (ϕ_1 and ϕ_2) and the saturated permeability values (k_1 and k_2) of micro-porous regions, using the total permeability (K) value as well as the macro-porosity (ϕ_0) and the permeability of the macro-pores (k_0) as input parameters. For the current work, we have segmented the un-resolved pores into only two micro-porous phases. A multi-modal deep learning model is implemented in PyTorch with two input branches and one output branch. One of these input branches processes the input parameters (K , ϕ_0 and k_0) while the other branch processes the geometry of the porous media in the form of 2D images. The outputs from these two branches are concatenated together as a single feature map which is then further processed by the output branch to predict the desired output. An illustration of the model is presented in the graphical abstract. The data for training and evaluating the model has been generated through multiscale pore network modelling using the extensive pore modelling (XPM) simulator. The voxel-based XPM simulator computes the multi-phase characteristics of the digital rock volumes by incorporating the flow properties of the unresolved phases.

The model was able to predict the micro-phase properties, albeit with varying accuracy. For the 14.6% of the test cases, the porosities and permeability values of both micro-porous phases were correctly predicted within a margin of $\pm 15\%$. For the 59.2% of the test cases, the porosity and permeability of only one of the micro-porous phases were correctly predicted within the margin of $\pm 15\%$. Upon close examination of these test cases, it was observed that the incorrectly predicted phase may not have contributed to the overall flow and can be considered as solid grains. The properties of both the micro-porous phases were incorrectly predicted for the remaining 26.2% of the cases. In this case, the discrepancy may be attributed to the under-segmented images and for these cases, we may require more than two micro-porous phases. In this work, we have shown that deep learning models can be utilized to characterize the unresolved micro-porosity. We intend to extend this model to predict the multi-phase characteristics of the micro-porous phase in future.

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MS04 / 436

Evaluating Physiochemical Properties of Expansive Soils through Electrokinetic Conditioning

Author: Najibullah Zulfeqar¹

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This study focuses on the electrokinetic conditioning of expansive soils, emphasizing the physiochemical aspects –an area frequently overlooked in prior research. Expansive soils, known for their propensity to swell and shrink in response to moisture fluctuations, present formidable challenges

in geotechnical engineering. These volumetric alterations can lead to soil heave and settlement, jeopardizing the stability of structures built upon them. Electro-kinetic soil conditioning offers a cost-effective, easy-to-implement, and less destructive approach to rapidly stabilize expansive soils under the existing infrastructure, such as pavements and road systems. Ion exchange, chemical transport, and cementation occur near the electrodes during electro-kinetic soil stabilization. Electrokinetic treatment condition was performed on a high plasticity soil, under constant electric field intensities of 67, 100, and 167 V/m, to investigate induced chemical and microstructural changes. A decreasing current was observed during the 7-day conditioning period. Soil pH analysis revealed an acidic region zone near the anode and an alkaline region near the cathode, resulting from water electrolysis reactions. The electric conductivity of the soil increased near the anode while decreasing toward the cathode. X-ray diffraction was unable to distinguish any mineralogical changes in the soil. However, scanning electron microscopy revealed microstructural alterations, including desiccation and void formation near the anode, dense particle aggregation near the cathode, and intermediate changes in between. These findings elucidate the complex processes occurring during electrokinetic soil conditioning, informing optimization strategies by controlling voltage, electrode materials, and treatment time for effective expansive soil stabilization. This finding could offer invaluable insights into its capacity to modify expansive soil properties and mitigate the soil's swelling and shrinkage propensity.

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Poster / 437

Tracking Biomineralization in Shale Fractures with Magnetic Resonance Velocimetry (MRV) and Computed Microtomography (Micro-CT)

Author: Matthew Willett¹**Co-authors:** Sarah Codd¹; Dustin Crandall²; Joseph Seymour¹; Adrienne Phillips¹; Catherine Kirkland¹¹ Montana State University² National Energy Technology Laboratory**Corresponding Authors:** catherine.kirkland@montana.edu, jseymour@montana.edu, adrienne.phillips@montana.edu, matthewwillett@montana.edu, scodd@montana.edu, dustin.crandall@netl.doe.gov

Meeting ambitious carbon neutrality goals set by governments worldwide requires a multifaceted approach. One area of focus is the utilization of subsurface energy resources, particularly in shale formations located thousands of feet underground. Although this reservoir was an important contributor to the natural gas boom of the 2000s, it has increasingly been explored for other, more environmentally sustainable processes such as CO₂ sequestration [1, 2], geothermal energy [3, 4], and hydrogen geo-storage [5]. However, a key concern with these applications is fractures that arise in shale, which could potentially lead to buoyancy-driven migration of greenhouse gases and valuable energy resources [6]. One solution to enhance shale integrity is biologically engineered mineral precipitation, also known as microbially-induced calcium carbonate precipitation (MICP) [7]. An early study showed that elevated pressures (6.12 MPa) do not hinder biomineralization in

fractured shale, with up to four orders of magnitude permeability reduction achieved [8]. Follow-up research demonstrated that MICP treatment was similarly successful at sealing fractured shale cores at elevated temperatures (60°C) [9, 10]. Although these studies showed that subsurface conditions are favorable environments for precipitation, they called for further analysis to better understand fluid-rock interactions integral for sealing.

On the reservoir scale, a ‘cubic law’ model derived from the Reynolds equation and lubrication theory is often used to approximate flow fields based on an average fracture width [11, 12]. More accurate ‘local cubic law’ (LCL) models can calculate local flows based on the local aperture, which can be measured by highly detailed computed microtomography (micro-CT) scans of the fracture [13]. Alternatively, magnetic resonance velocimetry (MRV) can be used to experimentally measure fluid quantities in opaque systems non-invasively in 3D [12, 14, 15]. By combining spatial encoding (k-space) with molecular displacement measurements (q-space), velocity maps can be measured for various flow types, including flow through porous media. Spatial information can also be sacrificed to obtain a probability distribution of molecular displacements called a propagator, which offers high temporal resolution with respect to changes in flow and pore structure [16].

This study represents the first application of MRV to visualize and investigate fluid flow in shale fractures. Velocity maps and propagators characterize flow within fractured shale cores (5.08 cm length, 2.54 cm diameter) and track changes in pore structure and flow fields due to MICP-treatment (Fig.1). Complementary micro-CT imaging reveals changes in fracture aperture maps and fluid flow from LCL simulations. The results show that mineral formation due to MICP changes preferential flowpaths and confirm that MRV is an effective tool for tracking sealing progress in rock fractures, providing invaluable information for optimizing MICP injection strategies and fluid flow numerical simulations for advancing subsurface energy applications.

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MS13 / 438

Electrosorption-induced deformation of microporous carbons: molecular dynamics and mean-field theory

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Nanoporous carbons play an important role in different electrochemical applications and, in particular, are widely used as porous electrodes in super-capacitors. Ions in aqueous electrolytes form the electrical double layer on the charged electrode-solution boundary, which can lead to a complex physical picture in nanosized pores. In this work, using molecular dynamic simulations and the framework of the modified Poisson-Boltzmann equation [1], we studied the structure of the electrical double layer and the developed solvation pressure in slit graphitic micropores immersed into a 1:1 aqueous electrolyte. Namely, we used NaCl aqueous solution, as one of the most common. We focused on the behavior of solvation pressure as a function of pore width and surface charge density. Two different water models were used: explicit one –based on SPC/E [2] water molecule and implicit one, i.e. structureless background with fixed dielectric permittivity. The latter allows us to perform the most accurate comparison between molecular dynamics and theory. We demonstrated that the theory could predict the solvation pressure dependence on the pore width almost quantitatively correctly compared with the results using the implicit water model. In turn, the simulations with explicit water show the qualitatively different behavior of the solvation pressure in 1 nm and 2 nm pores as a function of surface charge density. We demonstrated that the value of the solvation pressure is defined by a delicate balance between Van der Waals and electrostatic contributions. Finally, using the theoretical approach we estimated the solvation pressure on the macroscopic scale using earlier developed approach [3], which have been developed to describe adsorption-induced deformation. Our results can be used in the further development of a theoretical framework for the description of electrosorption-induced deformation.

Country:

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Water & Porous Media Focused Abstracts:

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Poster / 439

Understanding the Time-Dependent Deformation of Microporous Carbons Due to Adsorption

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Equilibrium and kinetic behavior of adsorption-induced deformation attracted much attention in the last decades [1,2]. This phenomenon is ubiquitous but challenging to predict quantitatively due to numerous factors (pore size and geometry, adsorbent/adsorbate combination, temperature, etc.) affecting its manifestation. Time may be considered as one of these factors as many industrial and real-world processes occur far from thermodynamic equilibrium. The theoretical and experimental works cover activated carbons, coals, zeolites, glasses, etc. However, most of the theoretical works are focused only on the equilibrium part of the deformation process or only on the description of the time evolution of the adsorption process. The present contribution [3] aims to cover the existing gap, using the combination of two theoretical frameworks: the diffusion-based description of the time-dependent adsorption process and the osmotic ensemble-based description of adsorption-induced deformation. We obtained self-consistent equations describing equilibrium and out-of-equilibrium adsorption as well as deformation processes. As a next step, we verified the obtained equations on the experimental data [4] of carbon dioxide and methane on activated carbons (AC Chemviron and AC T-3). Our results demonstrate that the model can describe both equilibrium and kinetic adsorption and adsorption-induced deformation data. Also, we considered the possible influence of slow relaxation processes in the adsorbent on the adsorption process. We showed that at low strain relaxation rates, the diffusion process is hindered by deformation. On the other hand, at high strain relaxation rates, the deformation process is defined by the local adsorbate concentration and “follows” the diffusion. The current work helps to interpret experimental data on time-dependent adsorption-induced deformation.

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MS01 / 440

The Impact of Carbon Dioxide- Methane Co-Injection into Deep Saline Reservoirs: A Case Study from the Otway Storage Site

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The injection of CO₂ into deep saline reservoirs is an important greenhouse gas mitigation strategy. In many cases, the CO₂ source is made up of a mixture of different greenhouse gases. One such case is at the Otway International Test Center in Australia, where the source of CO₂ comes from a natural gas reservoir made up of a mixture of methane (CH₄) and CO₂. Both CO₂ and CH₄ are soluble in water, though CO₂ is about an order of magnitude more soluble than CH₄. In this work, we consider how that difference in solubility affects the transport of CO₂ and CH₄ away from the injection well using analytical solutions and numerical simulation. We find that injecting a mixture of CO₂ and a modest fraction of CH₄ results in a methane bank forming at the beginning that grows over time as the plume migrates. The results of this work can be used to inform project decision-making and monitoring plans for future projects that inject a mixture of CO₂/CH₄ into a saline reservoir.

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MS25 / 441

Experimental Study on Carbon Mineralization in Fractured Basalt using X-ray CT imaging

Authors: Woojae Jang¹; Tae-Hyuk Kwon¹

Co-authors: Gyeol Han²; Hyun-Woo Joo³; Marcopolo Alcantara Fuentes¹; Jeonggyu Seo⁴; Jaehan Park⁴; Jihyuk Kim⁴; Hosang Kim⁴

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Carbon mineralization is a promising method of geological carbon storage since it enables safe storage on a short time scale, which typically requires a long time when supercritical CO₂ is stored. Basalt is considered a potential host rock formation for carbon mineralization, as it is abundant globally and located at relatively shallow depths, providing advantages in terms of capacity and

injectivity. Moreover, it contains a substantial amount of divalent cations, which allow rapid reaction kinetics. This study conducts two carbon mineralization tests by injecting a supersaturated and slightly alkaline solution into two fractured basalt cores at a flow rate of 1 and 5 mL/min. The saturation index and pH of the injected solution were approximately 0.4 and 7.2, respectively, representing the far-field condition where precipitation dominantly occurs. During the approximately 40 days of injection, several X-ray CT scanning and permeability tests were performed for both mineralization tests. X-ray CT imaging revealed that more calcite precipitated when applying high flow rate than low flow rate. This is because a greater amount of reactive solution was transported into the fracture for the same injection duration. For the high flow rate test, the calcite evenly precipitated along the entire fracture surfaces, whereas, under low flow rate, preferential precipitation was observed near the inlet. Preferential precipitation occurred because the low flow rate provided sufficient retention time relative to the reaction kinetic. Comparison to obtained relationship between permeability and porosity to the Kozeny grain-coating model indicates that the empirical parameters n ranges from 80 to 100 at the high flow rate, whereas it ranges from 100–120 for the low flow rate test. The difference means that the extent of permeability reduction was more significant for the same amount of precipitation due to local clogging. 1-D numerical solutions of advection-diffusion-reaction also reveal that a flow rate of 1 mL/min results in the local clogging for the condition similar to the flow tests. The results of this study imply that when a low flow rate is applied relative to the precipitation kinetics in actual carbon mineralization field, local clogging may occur, subsequently leading to a decrease in injectivity and capacity.

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MS25 / 443

Pore scale experimental and computational analysis of reactive transport in a natural limestone

Author: Hongkyu Yoon¹

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Reactive transport processes in porous media have a significant impact on many subsurface energy activities including in-situ, ex-situ carbon sequestration, long-term performance of enhanced geothermal systems, geologic hydrogen storage, unconventional resources recovery among others. Over the past two decades, our understanding of pore-scale reactive transport processes has been dramatically improved through both experimental and computational studies (e.g., Yoon et al., 2015; 2019). In this work fluidic systems made of a natural limestone are used to evaluate reactive transport processes including dissolution and precipitation. A wide channel system on the surface of the limestone is used to evaluate the impact of different influent solution chemistries over pH and ion species on chemical reaction rates, reaction feedback on hydrodynamics, and their coupling process. The reactive flat surface is characterized for surface roughness and elemental/mineralogical mapping is performed after experimental works. During reactive transport experiments reactive surfaces are monitored using optical and confocal microscopy as well as analysis of effluent solution. A hybrid lattice Boltzmann-finite volume (LB-FV) approach for reactive transport including dissolution and precipitation processes is used to analyze experimental observations. To improve computation efficiency dramatically a GPU-based LB simulation will be employed to account for hydrodynamics

and machine learning-based model (e.g., convolutional/artificial neural networks) for chemical reaction speciation will be developed and applied for reactive transport processes. In this presentation we will highlight how experimental observations including dissolution and precipitation through imaging and solution chemistry can be utilized to validate pore scale modeling to improve our understanding of calcium carbonate precipitation and dissolution processes in the natural limestone. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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Poster / 445

Enhanced hydrocarbon removal from porous media: pore-scale investigation using polymer and alcohol solutions

Authors: Bakbergen Bekbau^{None}; Dinara Turalina^{None}; Sagyn Omirbekov¹; Zhansaya Aitkhozha^{None}

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Abstract

Soil pollution by petroleum hydrocarbons a global environmental problem with harmful effects on ecosystems and human health. Remediation is an essential for restoring soil quality and preventing further environmental degradation.

Petroleum hydrocarbons, including crude oil and its derivatives are composed of petroleum hydrocarbons that can remain in the soil for an extended period, making conventional remediation approach difficult. Current methods, including bioremediation or physical removal, can be slow or costly and aren't suitable for larger-scale or deep contaminations. Recent studies have explored innovative solutions involving chemical agents, including polymers and alcohols, to enhance pollutant displacement and solubilization, improving remediation efficiency [1–3].

This study addresses the challenge of efficiently removing petroleum products from contaminated pore structures using polymer solutions enhanced with alcohols as agents for sweeping and dissolution. We also investigate the impact of wettability, alcohol/polymer concentration, and the geometry of porous media on remediation performance. To support our analysis, we utilize AI-specialized software for image post-treatment, enabling precise visualization and quantification of hydrocarbon displacement within the soil structure.

The present study will provide insight into improving our understanding of, and fine-tuning the enhanced hydrocarbon remediation technique in porous media at a pore scale. This finding is distinct

from earlier methods, which utilized either polymers or alcohol alone. By combining these agents, we observe an enhanced synergistic effect that accelerates the removal of hydrocarbons compared to earlier methods. This finding opens up new possibilities for improving the effectiveness of soil remediation technologies.

Effective petroleum hydrocarbon removal at the pore scale can result in appropriate technology with greater cost efficiency, faster response timing, and lower risk of environmental consequences. Our results offer a framework to minimize such strategies to large scale contamination cleanup. Finally, the findings of this study hold implications for the wider arena of environmental contaminants and their remediation, highlighting the value of creative multidisciplinary approaches in addressing intricate environmental issues. The combination of polymers and alcohols could be a promising direction for tackling other forms of persistent contamination, further advancing environmental sustainability.

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446

Linking evolution of preferential flow paths, transport self-organization and chemical weathering in porous media using non-equilibrium thermodynamics

Authors: Erwin Zehe¹; Evgeny Shavelzon²; yaniv edery³

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We apply non-equilibrium thermodynamic framework to analyze the coupled reaction-transport interaction of reversible dissolution-precipitation of calcite, characteristic to the emergence of preferential flowpaths in subsurface geophysical systems. The reaction-transport interaction is modeled on a Darcy-scale using Lagrangian particle tracking, capable of capturing the multiscale heterogeneity phenomena. Dissolution-precipitation of calcite is driven by the injection of an acid compound into the porous matrix, initially saturated with resident fluid. We analyze the entropy production attributed to various dissipative processes in the field to describe evolution of preferential

flowpaths and the accompanying dissipative dynamics within the non-equilibrium thermodynamic framework.

The reactive-transport interaction enhances the emerging preferential flowpaths, leading to transport channelization, as attested by the Shannon entropy, and a decline in the normalized entropy production due to percolation and chemical reaction, signifying the decrease in reaction intensity and frictional dissipation. This is attributed to the intensification of transport channelization in the field due to the bounding of reaction within these paths, thus providing conductive channels for the flow which are preferable energetically. The flip side of transport channelization is the decline in the mixing of reactive species, corresponding to intensification of concentration gradients. This allows the interpretation of results as the evolution of a non-equilibrium system towards a stationary state under the applied constraint of influx of reactive species. This asymptotic stationary state corresponds to complete channelization of the medium, thus minimizing the mixing of reactive species, reducing the ensuing chemical reaction and providing energetically preferable conductive paths for the flow.

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MS11 / 447

Microfluidic investigation of water-scCO₂ phase distributions in vesicular basalt pore system proxies

Author: Tianxiao Shen¹

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In this study, we conducted a series of microfluidic experiments using Stereolithography (SLA) 3D-printed chips designed to replicate the pore geometry of vesicular basalts and investigate a scaled version of in-situ supercritical CO₂ (sc-CO₂)/water/basalt multiphase flow dynamics under room conditions and a large parameter space. Multiphase flow phase distributions will impact scCO₂ dissolution, reactant mixing paths, carbonate growth patterns, and relative permeability during sub-surface supercritical CO₂ injection for carbon storage and mineralization. Multiple field-scale pilot projects, such as those conducted at Wallula and CarbFix, underscore the viability of sequestering sc-CO₂ in basaltic formations, specifically in the highly permeable flow-top vesicular zones. These zones are characterized by millimeter-sized vesicles connected through microfractures across basalt matrix and nanopores in clay, forming a dual-porosity system with a large aspect ratio that differs substantially from conventional sedimentary reservoirs. The transport of sc-CO₂ under in-situ

conditions in basalt dual-porosity networks remains poorly understood, hindering accurate predictions of CO₂ migration and mineralization inside basaltic formations. To approximate these pore morphologies, each microfluidic chip features an interconnected channel network that mirrors the high-aspect-ratio pore structure and dual-porosity characteristics of vesicular flow-top basalts. To approximate in-situ fluid properties, we screen through combinations of fluorinated hydrocarbons as the nonwetting phase and glucose–water solutions as the wetting phase, effectively preserving the high viscosity ratio and wettability conditions of in-situ sc-CO₂/water/basalt systems under room conditions. Wetting and non-wetting fluids are co-injected by a syringe pump at various controlled rates and volume ratios to represent a range of reservoir conditions (i.e., flow rate and saturation state) from near-wellbore to far-field region. Bubbles of non-wetting fluid are generated through a T-junction at the inlet with a uniform size distribution controlled by channel width and flow rate. The dynamic evolution of bubbles within the interconnected channel system, including snap-off and coalescence events, are traced in the acquired video with AI-assisted image analysis. A U-shaped manometer is integrated at the inlet and outlet ports to measure the pressure differential across the chip, enabling the calculation of relative permeability of each phase under different flow regimes. These combined flow visualization and pressure measurements yielded critical insights into: (1) the feedback loop among CO₂ bubble size distribution, occurrence of snap-off/coalescence events, and relative permeability, (2) steady-state partial water saturation within both mobile and immobile fluids, and (3) the preferential flow pathways in dual-porosity pore systems analogous to vesicular basalts.

We posit that the presented microfluidic diagnostics will enable scalable insights into in-situ sc-CO₂ migration and phase distributions and, ultimately, mineralization behaviors within basaltic formations. Preliminary results suggest that flow rate and initial bubble size strongly influence local partial saturation, relative permeability, and bubble behavior. Looking forward, our work will extend toward incorporation of nanoporous materials and reactive minerals into the current chip design to better represent geochemical processes inside vesicular basalts. This expanded approach aims to elucidate the interplay between fluid transport, geochemical reactions, and dual-porosity nature, ultimately optimizing injection schemes for efficient and secure in-situ carbon mineralization in basaltic formations.

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MS15 / 448

Deep Learning Prediction of Reactive Dissolution in Porous Media

Author: Hannah Menke¹

Co-authors: Ahmed H. Elsheikh¹; Alhasan Abdellatif¹; Florian Doster ; Julien Maes¹; Marcos Cirne¹

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Reactive dissolution of solid minerals in porous media is a critical process underlying numerous subsurface applications, including carbon capture and storage (CCS), geothermal reservoir management, and oil & gas recovery. However, direct numerical simulators for modelling reactive flow and mineral dissolution often prove computationally prohibitive. To address this challenge, deep-learning methods - commonly based on convolutional neural networks (CNNs)—have emerged as promising alternatives. Yet, existing data-driven approaches typically focus on predicting velocity fields, overlooking the temporal evolution of rock structure during dissolution.

In this study, we introduce a novel deep-learning framework that integrates both spatial and temporal information to forecast the future states of a dissolving porous medium at a fixed time-step horizon. By leveraging sequences of past states as input, our method accurately captures the evolution of pore structure and mineral dissolution over time. When benchmarked against traditional numerical simulators and state-of-the-art data-driven methods, our approach demonstrates both higher predictive accuracy and remarkable computational efficiency. Notably, it achieves a speedup of approximately 10^4 compared to conventional numerical solvers, offering a powerful tool for large-scale, time-dependent simulations in the porous media community.

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MS07 / 449

Phase-Field Fracture Propagation in Thermo-Hydraulic-Mechanical Systems

Author: Mary Wheeler^{None}

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This presentation introduces a diffraction-based thermo-hydraulic-mechanical (THM) model for fracture propagation using a phase-field fracture (PFF) approach. The THM-PFF model integrates four primary solution variables—displacements, phase-field, pressure, and temperature—each governed by distinct principles: conservation of momentum (mechanics), a variational inequality (constrained minimization), mass conservation (pressure), and energy conservation (temperature). This results in a novel coupled variational inequality system. The system is sequentially solved based on the fixed stress iteration, for displacements, phase-field, pressure, and temperature in a staggered manner. The model features global coupling of pressure and temperature across the domain via diffraction systems, where diffraction coefficients are determined by material parameters weighted by the diffusive phase-field variable. To ensure robust local mass and energy conservation, enriched Galerkin finite elements (EG) are employed for the pressure and temperature diffraction equations. By enriching continuous Galerkin basis functions with discontinuous piecewise constants, EG accurately captures solution and parameter discontinuities while preserving local conservation laws—critical for realistic THM simulations. In addition, a predictor–corrector local mesh adaptivity scheme is implemented, enabling the model to handle small phase-field length-scale parameters with high numerical accuracy and computational efficiency. These advancements in modeling and algorithm

design represent a significant contribution to the field and are validated through rigorous numerical experiments.

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MS09 / 450

Depth-integrated model of immiscible two-phase flow in open rough fractures

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Immiscible two-phase flows in geological fractures are relevant to various industrial contexts, including subsurface fluid storage and hydrocarbon recovery. Direct numerical simulations (DNS) of first-principle equations, which resolve three-dimensional (3-D) fluid-fluid interfaces, can address various flow regimes but are computationally intensive. To retain most of their advantages while reducing the computational cost, we propose a novel two-dimensional (2-D) approach based on depth-integrating the 3-D first principle equations over the local fracture aperture. Such existing models have, so far, been restricted to single-phase permanent flow in rough fractures [1,2] and two-phase flow in 2-D porous media [3]. Considering a description of two-phase flow relying on the Navier-Stokes equations coupled with the volume-of-fluid method for interface capturing, we derive a depth-integrated model based on the lubrication approximation and assuming a parabolic out-of-plane velocity profile. Wall friction and out-of-plane capillary pressure are incorporated as additional terms in the 2-D momentum equation. The model then relies on a geometric description reduced to the fracture's aperture field and mean topography field. Implemented in OpenFOAM, it is validated against experimental [4] and 3-D DNS simulation results [5] for viscous fingering in a Hele-Shaw cell, and subsequently applied to a synthetic geological fracture geometry over a wide range of capillary numbers (Ca). With a tenfold reduction in computational cost compared to 3-D DNS, the model accurately predicts key flow metrics, such as macroscopic pressure drops and various statistical observables of the fluid displacement morphologies. The 2-D model performs best at intermediate Ca, demonstrating a potential for bridging hydrodynamic and continuum-scale models.

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Insights into Geochemical Processes of CO₂ Mineralisation in Basalts

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The geological storage of CO₂ in basalt formations has emerged as a promising solution for long-term carbon sequestration, leveraging the rapid reaction kinetics and high divalent cation content of basaltic rocks (Gislason et al, 2014 & 2018, Kelemen et al, 2019). Through the process of carbon mineralisation, injected CO₂ reacts with minerals such as plagioclase feldspar and pyroxenes to form stable carbonates, including calcite (CaCO₃), magnesite (MgCO₃), and siderite (FeCO₃) (Gislason and Oelkers, 2014; Matter et al., 2016). Carbon mineralisation ensures permanent carbon storage while utilising one of Earth's most abundant igneous rock types. However, uncertainties persist around mineral dissolution rates, secondary phase formation, and the stability of the precipitated carbonates under reservoir conditions relevant to basalt formations.

In this study, we conducted 38 high-pressure, static batch experiments to evaluate the geochemical behaviour of three different basalt rocks (Hawaiian Tholeiitic Basalt, Samson's Ribs and Cruick's Quarry), representing various ages and levels of alteration, in the form of powder under CO₂-rich conditions. The experiments examined the effects of particle size (<0.355 mm, 0.355–1.4 mm, and 1.4–3.35 mm), pressure (150, 350, and 750 psi), salinity (0, 35, and 100 ppt NaCl), and basalt type on dissolution and precipitation processes at 80°C. Analytical analysis including ICP, pH and conductivity measurements were performed to assess the interplay of primary mineral dissolution and secondary precipitation to uncover key mechanisms influencing the efficiency of carbon mineralisation.

Results demonstrate that smaller particle sizes significantly enhance dissolution rates by increasing reactive surface area, leading to elevated release of Ca, Mg, and Si. Conversely, larger particles facilitate secondary precipitation, particularly silica, due to localised oversaturation. Elevated pressures (750 psi) enhanced Ca and Mg dissolution relative to lower pressures, emphasising the role of pressure in driving reaction kinetics (Oelkers et al., 2008). Salinity exhibited a dual effect: higher salinities suppressed dissolution due to ionic strength effects, while lower salinities favoured Mg and Si release, aligning with previous findings (Fischer et al., 2019). Mineralogical variation among basalt types was a control parameter on the level of reactivity demonstrating that even older basalt rocks which have been exposed to natural processes can still work as good sites for storing carbon.

Correlations between pH, conductivity, and elemental release highlight the dynamic nature of geochemical interactions. Low pH values enhanced dissolution of reactive elements, while increased conductivity reflected cumulative ionic contributions. Secondary mineral precipitation trends, such as silica under alkaline conditions and carbonates under CO₂-rich environments, were consistent with predictions from prior studies (Carroll et al., 2013; Matter et al., 2016).

This research enhances the understanding of basalt's potential for CO₂ sequestration, demonstrating that even older basalts, despite significant alteration, can still serve as viable storage sites. This finding could significantly expand the possibilities for in situ mineralisation carbon storage. Therefore, it is essential to adopt a comprehensive site selection approach to ensure optimal storage conditions to accelerate mineralisation processes. Future work will involve integrating advanced geochemical modelling with experimental findings to refine reaction mechanisms and predict long-term system behaviour.

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MS23 / 452

Underground hydrogen storage from nano-scale to micro-scale

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To reduce carbon emissions, transitioning the energy system from traditional fossil fuels to clean energy sources is crucial. Hydrogen energy has emerged as a highly promising clean energy option, attracting increasing attention. However, one of the primary challenges hindering the development of hydrogen energy is its storage. Underground hydrogen storage (UHS) has become a vital technology for achieving large-scale, long-term hydrogen storage. Despite its potential, limited experience with UHS projects has left the mechanisms of hydrogen storage, transport, and leakage within

reservoirs inadequately understood. This study investigates the storage and flow characteristics of hydrogen in UHS from nano-scale to micro-scale. At the nano-scale, molecular dynamics (MD) simulations are employed to examine the adsorption behavior of hydrogen. The effects of temperature, pressure, and pore size on hydrogen adsorption in narrow slits of clay minerals are analyzed. Key findings include the distribution characteristics of hydrogen in slits, the amount of excess adsorption, diffusion coefficients, and gas-solid interaction energies. At the micro-scale, digital rock and computational fluid dynamics (CFD) methods are utilized to explore hydrogen flow behavior. Factors such as wettability and the capillary number are analyzed for their effects on hydrogen storage and recovery efficiency during multiple hydrogen injection and recovery cycles. This study elucidates the mechanisms of hydrogen storage and transport from a microscopic perspective, offering valuable insights for predicting hydrogen transport and distribution in UHS. Furthermore, it provides a theoretical foundation and technical support for advancing underground hydrogen storage technologies.

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Poster / 453

Induced Seismicity Event Detection using Multi-station Time-frequency-Based Machine Learning Models at a geologic carbon storage site

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Early detection and monitoring of induced seismic events resulting from geologic CO₂ injection is crucial for ensuring the safety and stability of geologic carbon storage (GCS) operations. At many GCS sites, passive microseismicity detection and analysis is tedious and proper design of autonomous detection systems is labor-intensive. In this study we use multi-head convolutional neural networks (CNNs) to detect microseismic activity induced during GCS from continuous recordings at the Illinois Basin Decatur Basin (IBDP). Multi-channel spectrograms (i.e., time-frequency images) from deep borehole and surface sensors are used as inputs to multi-head CNN models. Conventional pickers are also used to make a labeled data for both p- and s-arrival times, which are used as a reference case to evaluate the performance of machine learning models. In addition, we utilized energy-related features of waveforms such as Mel-frequency Cepstral Coefficients and/or multi-level output from wavelet decompositions. These features were selected based on feature identification through decision-tree based analysis. Preliminary analysis shows the addition of these features enhances the accuracy of event detection, but more waveform data from different sensors such as geophones within the reservoir, above reservoir, and surface array is a primary factor to improve coverage and enhance detection. We will demonstrate how the usage of spectrogram and proper data normalization for pre-processing enables us to improve event detection even with limited data availability. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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455

The effect of gas mixing on the performance of hydrogen storage in depleted gas reservoirs

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Renewable energy production is gaining significant attention worldwide as a preferred alternative to fossil fuel-based energy sources, driven by the need to meet international climate protection agreements. However, the seasonal and intermittent nature of renewable energy generation requires large-scale energy buffers to manage energy imbalances. Hydrogen as a clean energy carrier and its underground storage offer a promising solution to overcome this challenge. Nevertheless, the flow behavior of hydrogen in porous rocks and its in-situ mixing with indigenous gases in the reservoir should be studied to improve hydrogen recovery factor, purity, and energy efficiency. This paper introduces an interpolation technique to model the effect of mixing of hydrogen and the in-situ gas in the storage reservoir on the performance of underground hydrogen storage. This interpolation technique incorporates the effect of mixing on the relative permeability of hydrogen and the resident gas based on the mole fraction of hydrogen in the mixing zone. The suitability of the new relative permeability relation is demonstrated using field-scale numerical simulations. The results show that neglecting the effects of gas mixing (even in a homogeneous rock) leads to overestimating hydrogen purity by approximately 5.3% and final hydrogen recovery by more than 3.4%. The results of this study can be used to improve the reliability of underground hydrogen storage modeling, and reservoir management.

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MS07 / 456

Advancing constitutive models for expansive clays: integration of suitable effective stress and water retention frameworks

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Expansive clays, such as bentonite, are involved in the design of engineered barriers for municipal and nuclear waste disposal. These materials are characterized by very low permeability, high swelling capacity, and self-healing properties, which ensure effective waste isolation and long-term stability under many different environmental conditions. Given the critical nature of their engineering applications, the design and use of these engineered barriers demand an accurate prediction of their behaviour. Although these materials have been employed in such roles for many years, the tools currently available and the physical understanding of the phenomena governing their behaviour remain limited, posing significant challenges to their application. This study introduces a novel stress-strain constitutive framework to simulate the behaviour of compacted bentonite under varying environmental loads, such as changes in relative humidity and mechanical loads at different saturation levels. Based on the physical behaviour of the material, the proposed formulation integrates the Advanced Constitutive Model for Environmental Geomechanics (ACMEG) with a water retention framework that distinguishes between capillary and adsorption mechanisms based on microstructural observations from the literature. Key advancements include a compaction-dependent air entry suction for the Capillary Water Retention Curve (CWRC) and an interaction function that accounts for hydration and compaction states of the material. Furthermore, an innovative effective stress formulation incorporates electrochemical stresses taking place from the interactions between clay particles and pore water molecules. The constitutive model is validated on a single Gauss point through simulations of uniaxial consolidation, isotropic compression under varying suctions, and constant-volume wetting tests at different dry densities on a MX-80 bentonite. Results demonstrate the ability of the model to capture the mechanical behaviour across a wide suction range and accurately predict swelling pressure under different compaction states. This work contributes to providing a robust tool for the analysis and optimization of engineered barriers, addressing critical gaps in current constitutive approaches.

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MS01 / 457

Experimental Investigation of Mineral Precipitation Dynamics in Porous Media and Its Impact on Rock Properties

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Mineral precipitation in porous media can significantly alter essential rock properties such as porosity and permeability, which are crucial for subsurface applications including geothermal energy production, CO₂ storage, and water resource management. This study utilizes XRCT-assisted core flooding experiments to systematically track the development and propagation of the mineral precipitation front, analyzing its effects on rock properties over time. We also measure seismic velocities at various stages of the experiment to dynamically assess changes in the medium's elastic properties as mineral precipitation progresses.

High-resolution XRCT imaging reveals the variability in mineral morphology influenced by flow conditions within the pore space, highlighting the complex interplay between geochemical reactions and flow dynamics. Additionally, by linking variations in seismic response to different stages of mineral clogging, we explore the potential for using seismic data to infer clogging risks in subsurface environments. Our results offer valuable insights into how varying flow conditions dynamically influence rock properties and underscore the importance of integrating multiple experimental techniques for comprehensive analysis.

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MS06-A / 458

Mechanisms for Enhanced Mixing in Unsaturated Porous Media

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The coexistence of multiple immiscible fluids in porous media alters velocity distributions, creating dead-end regions and high-velocity channels that significantly affect solute transport, mixing, and reactivity in both natural and industrial systems. To investigate this at the pore-scale, we simulate the simultaneous flow of two immiscible fluids, air and water, using OpenFOAM. Our study includes a set of high-resolution, 2-D and 3-D numerical simulations in granular porous media. Multiple saturation degrees are simulated using a method that allows precise control over the desired saturation degree. Once the phases are stationary, we simulate conservative transport across a broad range of Peclet numbers. The resulting scalar field forms an advancing mixing front, which can be interpreted to predict mixing-limited reactions.

In this work, we primarily focus on the deformation of the mixing interface and pore-scale concentration fluctuations, which are widely recognized as key drivers for global reaction kinetics. Our analysis distinguishes between mixing in dead-end regions and transmitting pores, highlighting how trapping in dead-end regions becomes a significant mixing mechanism at lower water saturation levels. Furthermore, we observe that persistent concentration gradients in transmitting pores

significantly enhance interface deformation, further contributing to mixing. We develop and validate a theoretical model that quantifies the effects of solute trapping and mixing within dead-end regions, as well as mixing interface deformation in transmitting pores. Lastly, we evaluate the impact of dimensionality (2D vs. 3D) on mixing across different saturation levels, which is particularly important in unsaturated systems, where the connectivity of fluid phases in 2D flow domains is highly sensitive to saturation changes. Under the same unsaturated conditions and Peclet number, 3D systems show significantly less mixing enhancement than 2D systems.

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MS09 / 461

Anisotropic Permeability Prediction at the pore scale: A Lattice Boltzmann and Machine Learning Approach

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Understanding the directional properties of porous media is crucial for accurately predicting flow behavior, reactive transport, and fluid solid interactions in applications such as geothermal systems, energy storage devices, and biological systems. Directional permeability values, which reflect the medium's response to flow at various angles, are especially important for complex geometries with an inherent anisotropy. In this study, we used a Lattice Boltzmann (LBM) model to calculate directional permeabilities from porous media patterns with different angles of flow inlet.

Three classes of porous media were generated for this study: (1) media with circular grains, (2) media with elliptical grains, and (3) media combining circular and elliptical grains. For circular grains, we varied parameters such as grain diameter distributions, a number of circles, and inter-circular distances. For elliptical grains, we varied eccentricity, semi-major and semi-minor axes, and the number of ellipses. The mixed media combined features from both types. Our investigation primarily aims to analyze the anisotropy of porous media. Isotropic media theoretically permit permeability prediction in any direction via linear transformation from the principal direction. However, it is not thoroughly investigated in anisotropic porous media. Circular grains serve as a baseline for the isotropic geometry, whereas elliptical and mixed grains represent cases of anisotropy. Using our LBM flow model, permeability was calculated at 10° intervals across 360°, producing 36 data points per image of porous media. This approach generated a comprehensive dataset for the three media classes, each yielding unique functional relationships between angle and permeability.

We aim to train a machine learning model to predict permeability as a function of inlet flow angle

for a porous medium image input. We would be able to compare machine learning performance as response to three different classes of obstruction patterns. Additionally, we want to explore the feasibility of using linear transformations from the principal direction to estimate permeability in anisotropic media. Apart from these, we would study the effects of geometrical properties like eccentricity, radius, axis lengths on the relationship between permeability and angle of inlet for a same class of porous medium.

Our findings could significantly enhance the understanding of directional transport properties in porous structures, providing deeper insights into the impact of geometric anisotropy on flow behavior. Additionally, they could pave the way for developing more accurate and efficient predictive models for complex geometries, with potential applications in fields such as filtration, energy storage, and subsurface fluid flow. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS26 / 462

Sub-core Permeability Inversion of Sedimentary Rocks using Positron Emission Tomography Data—Sally's Vision 10 Years in the Making

Authors: Christopher Zahasky¹; Zitong Huang²

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Multiscale permeability parametrization in geologic cores is key for quantifying multiphase flow and conservative, reactive, and colloidal transport processes in geologic systems. Despite its importance in controlling flow and transport processes, permeability measurement methods often suffer from low spatial resolution, high computational cost, or lack of generalizability. This study leverages positron emission tomography (PET) experimental data to record time-lapse radiotracer concentration distributions at millimeter-scale resolution in geologic cores. Through iterative forward simulations, an Ensemble Kalman Filter (EnKF) is employed to assimilate the input transport data and an ensemble of possible permeability distributions to determine the corresponding three-dimensional permeability map for a given geologic core sample. A second approach, specifically a convolutional neural network (CNN) is also used for permeability inversion. This data-driven CNN eliminates the need for numerically defining and iteratively running a forward operator once the training is completed. The EnKF and CNN methods are separately evaluated for permeability inversion with a combination of synthetically generated data and PET imaging data. Inverted 3-D sub-core scale permeability maps are used to parameterize forward numerical models for direct comparison with the PET measurements for accuracy evaluation on experimental data. The trained CNN produces more robust inversion results with orders of magnitude improvement in computational efficiency compared with the EnKF. Finally, we propose an improved EnKF inversion workflow where the initial ensemble is generated by adding perturbations to the CNN permeability map prediction. The results indicate that the hybrid EnKF-CNN workflow achieves improvements in inversion accuracy

in nearly all core samples but at the expense of computational efficiency relative to the CNN alone. Overall, this combination of experimental, numerical, and deep-learning methodologies considerably advances the speed and reliability of 3-D multiscale permeability characterization in geologic core samples.

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MS05 / 463

Unraveling the Role of Bacterial Motility and Chemotaxis in Heterogeneous Concentration Fields within Porous Media

Authors: Maximilian Stoll¹; Marco Dentz²; Roman Stocker³; Joaquin Jimenez-Martinez¹

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Chemotaxis enables microbes to navigate nutrient gradients, playing a critical role in nutrient cycling, soil respiration, and the fate of contaminants in the subsurface. While understanding microbial interactions with nutrients and contaminants is essential, the influence of bacterial chemotaxis—particularly in relation to fluid flow—remains insufficiently explored.

This study investigates the intricate relationships between microbial behavior, hydrodynamics, and the physico-chemical properties of porous media. A microfluidic platform was developed to replicate subsurface microenvironments, incorporating hydrogels for controlled, diffusive nutrient release to mimic natural nutrient sources such as roots and soil aggregates. This platform allows real-time adjustments of chemical heterogeneity in the porous medium and provides optical access to monitor bacterial movement and fluid flow. Using this system, the effects of bacterial traits like motility and chemotaxis on nutrient exposure were analyzed, along with their influence on cell transport under varying flow conditions and porous medium heterogeneities.

The findings reveal the control that porous medium heterogeneity exerts on bacterial nutrient exposure and the value of motility and chemotaxis depending on the conditions.

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MS25 / 465

Stability of two-phase flow with interfacial flux in CO₂ mineralization: Theory for complex system evolution

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The primary objective of Carbon Capture and Storage (CCS) applications in porous media is to achieve a stable and planar CO₂ displacement front, thereby suppressing viscous fingering. Particularly, a stable front can ensure uniform and exhaustive carbonation throughout a reactive medium. Drawing inspiration from experimental observations of CO₂ flooding into cores of portland cement-based materials, we examine the stability of such systems. Focusing on the early injection time allows us to reduce the complex problem, typically involving thermo-hydro-mechanical-chemical interactions, into a two-phase flow scenario of immiscible displacement with an interfacial flux (from the invading CO₂ phase into the resident water solution). This simplification is then justified a posteriori.

The formulated equations with the interfacial flux term are used to investigate the development of a saturation profile and define a base-state solution for linear stability analysis. Assuming negligible capillary forces and a step-profile allows us to derive a closed-form stability criterion. Findings show that the interfacial flux can either suppress or promote perturbations depending on the saturation profiles, typically leading to stability enhancement. Implications are then briefly drawn. Finally, this research demonstrates the important role of theory in simplifying complex multi-physical and scale processes and inferring the ultimate state of subsurface systems.

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Roded, R., & Dalton, L. E. (2024). Stability of two-phase flow with interfacial flux in porous media: CO₂ mineralization. *Physics of Fluids*, 36(11). <https://doi.org/10.1063/5.0237389>.

MS15 / 466

GenAI4UQ: A Generative AI Framework for Accurate and Fast State Variable Forecasting in Geological Carbon Storage

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Forecasting reservoir pressure and CO₂ plume distribution in geological carbon storage (GCS) demands the efficient integration of monitoring data with reservoir simulations. Traditional inverse modeling methods often rely on restrictive linear or Gaussian assumptions, limiting their predictive accuracy for complex state variables. Moreover, simulating large-scale three-dimensional (3D) GCS problems is computationally expensive, making iterative runs in inverse problems prohibitive.

To address these challenges, we propose GenAI4UQ, a software package designed for inverse uncertainty quantification in model calibration, parameter estimation, and ensemble forecasting. Powered by a conditional generative AI framework, GenAI4UQ replaces computationally expensive iterative simulations with a direct, AI-driven mapping. Its capabilities include rapid ensemble generation, robust uncertainty quantification, and efficient use of computational and storage resources. The software's automated hyperparameter tuning further ensures accessibility for users with diverse expertise levels.

We demonstrate the effectiveness of GenAI4UQ in forecasting 3D pressure and saturation fields during a 30-year CO₂ injection period. Our method achieves low root mean square error (RMSE) values, accurately capturing spatiotemporal distributions of state variables. Remarkably, GenAI4UQ generates 100 ensemble forecasts of 3D state variables in just 10 seconds, highlighting its unparalleled computational efficiency. Ensemble averages closely align with ground truth values, and the model effectively captures variability and observational noise, ensuring reliable uncertainty quantification.

By enabling rapid parameter distribution estimation and model predictions for new observations, GenAI4UQ equips researchers and practitioners with a powerful tool for real-time decision-making in GCS applications. This generative AI-based approach provides a practical and efficient solution to the computational and predictive challenges in large-scale GCS applications.

The code is available at <https://github.com/patrickfan/GenAI4UQ>

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MS19 / 467

A Film-Based Methodology for Simulating Electrical Properties in Digital Rock Samples

Author: Gabriel Machado dos Santos¹

Co-authors: Nicolao Cerqueira Lima¹; Thalís Otávio Siqueira de Oliveira¹; João Victor Bernardino Afonso e Silva¹; Antonio de O. Samel Moraes¹; Rodrigo Surmas²; Rodrigo Skinner²

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The resistivity index (RI) is a crucial parameter for characterizing the electrical properties of geological formations. Accurate measurement of RI is essential for understanding fluid distribution and behavior in porous rocks, with direct implications for applications such as hydrocarbon reservoir evaluation and enhanced oil recovery. These assessments are vital for optimizing resource extraction while minimizing environmental impact. Typically, the analysis of RI curves relies on the saturation exponent derived from Archie's law, which relates the electrical properties of rocks to their fluid saturation. Sandstone formations, in particular, often exhibit saturation exponents close to 2 due to their water-wet nature, which promotes the formation of water films at the rock-oil interface. As a result, analyzing RI under low water saturation conditions remains a significant challenge, as deviations in RI curves are commonly observed. These deviations are strongly influenced by the presence of those thin water films at the rock-oil interface, which significantly affect the overall conductivity of the system. In numerical simulations, most pore-scale fluid distribution methods do not account for the natural formation of these films, whereas more advanced methods capable of generating water films, such as numerical solutions for the fluid flow within the pore space, are computationally expensive and often impractical for large-scale simulations. Consequently, the electrical properties of these water films are often oversimplified or neglected in conventional modeling approaches, leading to discrepancies between modeled and experimental results.

In this work, we address these challenges by implementing a robust numerical simulation framework to calculate resistivity index curves for digital rock samples. This framework includes the development of a methodology that accounts for the presence of water films at the rock-oil interface. These water films are numerically introduced into the pore structure of the digital rock sample, enabling a more realistic representation under partially saturated conditions. A conductivity relation for the water films derived from the Langmuir equation is used to model the film conductivity as a function of film thickness and water conductivity. The resistivity index curves generated from simulations of different digital rock samples exhibited saturation exponents close to 2, aligning with empirical observations reported in the literature.

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MS26 / 469

Statistical Analysis of Cased-Hole Monitoring Well Logs for the GeoCquest Field Validation Experiment based on a Time-Lapse Technique: Interpretation Example and Interpretation Accuracy

Author: Aman Raizada¹

Co-authors: David Bason²; Mitch Allison²; Jeffrey Miles³; Yang Xingwang⁴; ZhanGuo Shi⁴; Catherine Spurin¹; Peter Cook⁵; Sally Benson¹

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The GeoCquest Field Validation (GFV) Experiment is a field-scale geological carbon sequestration research test conducted under the Otway Stage 4 program at the Otway International Test Centre, Victoria, Australia. The study involved the injection of approximately 10,000 tonnes of supercritical CO₂-rich gas (80 mol% CO₂ and 20 mol% CH₄) into the lithologically heterogeneous Paaratte Formation Parasequence 2 (PS-2) within the onshore Otway Basin at a depth of approximately 1.5 kilometers.

The GFV monitoring plan incorporated a strategically designed cased-hole pulsed-neutron logging (PNL) program, optimized for high temporal frequency and operational efficiency. This unique logging program was conducted in the newly drilled, dedicated passive monitoring well, CRC-8, over a period of 5 to 6 months. Data were collected with SLB's latest-generation pulsed-neutron instrument, the Pulsar service. Neutron-induced gamma ray counts are acquired as spectra in the energy and time domains, which are analyzed to yield Gas, Sigma, and Hydrogen-related measurements (GSH mode). For baseline runs, four passes of well logging were conducted in the eccentric configuration at a deliberately slow logging speed of approximately 200 ft/hr. The target Zone-of-Interest (ZoI) was an 80-meter interval within the freshwater aquifer that was initially saturated with brine. During the monitoring phase, up to three logging passes per day were performed under identical operational conditions.

The statistics of radiation counting were significantly improved by the slow logging speed and integration of daily passes, resulting in an excellent signal-to-noise ratio observed across both baseline and monitoring runs. This high-quality spatiotemporal PNL dataset enabled a rigorous statistical analysis of GSH measurements, examining their behavior on a depth-by-depth basis within the ZoI. The primary objective of the statistical study was to *detect* the presence of CO₂-rich gas at each depth point, sampled at 6-inch intervals, and to evaluate breakthrough times at CRC-8 with a *pre-defined confidence interval* (CI). Prior to analysis, PNL data were corrected for depth mismatches using automated depth alignment tools and in-house developed code to enhance precision in depth registration. An independent samples *t*-test was performed to compare the means of two independent groups: (1) the pre-injection baseline and (2) the daily monitoring data. The goal was to determine whether there was statistical evidence of a significant difference between the means of these groups, enabling the detection of CO₂-rich gas with a 95% CI at each sampling point. For depths where CO₂-rich gas was detected, saturation estimates were derived using a time-lapse interpretation technique. Furthermore, the uncertainty associated with these saturation estimates was quantified to improve the interpretation accuracy.

Our statistical analysis demonstrates a comprehensive evaluation of breakthrough times across multiple layers with a 95% CI. Breakthrough was observed as early as within a week, indicating the potential for gas migration through high-permeability streaks between the injector and monitoring wells, located nearly 100 meters apart. These findings highlight the effectiveness of the proposed methodologies in detecting and quantifying the migration of CO₂-rich gas in heterogeneous formations, providing valuable insights for advancing carbon sequestration monitoring technologies and improving the reliability of predictive models.

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Water & Porous Media Focused Abstracts:**References:**

MS25 / 470

Identification of a characteristic time and length for CO₂ mineralization**Author:** Vaughan Voller¹**Co-author:** Peter Kang²¹ *Department of Civil Environmental and Geo- Engineering, University of Minnesota, Minneapolis, MN 55455, USA*² *University of Minnesota***Corresponding Authors:** pkkang@umn.edu, volle001@umn.edu

Owing to its ubiquity and the complexities arising from the coupling of flow with reaction, mineral precipitation in porous media remains a continued area of research in reactive transport. An area of current focus is the mineralization of CO₂ in the subsurface. This is an attractive proposition because it allows for the secure and permanent sequestration of this greenhouse gas in subsurface reservoirs. In very general terms, this process involves the injection of a fluid charge, supersaturated in CO₂, into the pores of a rock reservoir. Initial, in the vicinity of the entrance to the reservoir, the charge dissolves the rock and mixes with the existing pore water. However, at the point where sufficient cations have been taken up and the pH of the charge has increased, precipitation of calcite minerals occurs. Here, our focus will be on CO₂ mineralization processes within rock masses that have relatively large values for the porosity and hydraulic conductivity. A particular target is basalts, with porosities in the range [0.05, 0.2] and hydraulic conductivities in the range [10⁻⁶, 10⁻⁵] m/s. Our expectancy is that CO₂ mineralization in such systems is controlled by the clogging of the pore spaces with the mineral product. This clogging will restrict the ability to deliver the CO₂ charge to the pore spaces at distances away from the reservoir entrance, eventually leading to complete clogging and shut-off termination of the operation. Within this scenario, our main aim is to arrive at a characteristic time and a characteristic length for the process, i.e., the time over which an effective operation can be sustained and the length (distance between input and output wells) that optimizes the storage potential of the reservoir. We achieve this by constructing a first order mineralization model that couples one-dimensional equations of porosity change, transport, and reaction. From this model we are readily able to identify a characteristic time scale for mineralization—essentially the earliest time for pore in the domain to clog. In addition, under the condition that flow through the domain is controlled by a fixed head drop, our model suggests the existence of a domain length that optimizes the storage, we propose that this an appropriate characteristic process length. A numerical analysis of the model identifies that a lower bound on this length can be obtained when the product of the hydraulic conductivity and head drop balances the mineralization reaction rate.

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MS14 / 471

An end-to-end multifidelity uncertainty quantification framework for CO₂-induced seismicity prediction in carbon storage sites

Author: Søren Taverniers¹

Co-authors: Herve Gross²; Hamdi Tchelepi¹

¹ *Stanford University*

² *TotalEnergies*

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In the quest to mitigate climate change, researchers have explored the geological storage of CO₂ in depleted oil and gas reservoirs, as well as deep saline aquifers. However, injecting CO₂ into these formations results in pressure buildup, which can lead to seismic activity, e.g., due to fault reactivation. Consequently, quantifying the risks associated with induced seismicity has become crucial. To systematically address this concern, we identify key input variables that impact quantities of interest (QoIs) relevant to seismicity. Using constitutive poroelastic relations and seismicity rate models, we propagate uncertainties in these inputs to corresponding uncertainties in these QoIs. We quantify this uncertainty propagation by adopting a Monte Carlo sampling approach to build cumulative distribution functions for the QoIs.

We present an end-to-end MC-based uncertainty quantification (UQ) framework for predicting the increase in seismic activity related to CO₂ injection in carbon storage sites. To speed up sampling, we use ideas from prior work on accelerated multilevel Monte Carlo for subsurface flow problems and from recent developments on devising optimal sample allocations for multifidelity Monte Carlo (MFMC) estimators. We deploy the resulting MFMC pipeline to estimate the cumulative distribution functions of relevant QoIs in CO₂-induced seismicity. Our approach uses simulations from the open-source simulator GEOS based on various levels of fidelity in terms of grid size and physical realism, along with predictions from data-driven approaches trained on GEOS simulations. We highlight some initial results demonstrating the end-to-end workflow and verify the correctness of our approach on a toy problem. Finally, we indicate next steps in applying our MFMC framework to real-world carbon storage sites.

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References:

MS01 / 474

Mixed-Dimensional Multiphase Model for Fractured Geothermal Reservoirs

Authors: Omar Duran¹; Veljko Lipovac¹; Inga Berre¹

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We present a novel multiphase compositional model for geothermal reservoir simulation that explicitly accounts for phase separation phenomena and the representation of fractures.

Mass and heat transfer simulations in porous media typically incorporate temperature as an independent variable alongside other natural variables. However, the implementation of these simulations can be complex due to the need for variable substitution procedures when modeling phase transitions. In contrast, the overall composition formulation does not require such substitutions, as it involves persistent equations and variables in every cell. For simulating brine and steam systems with high enthalpies, we employ the overall composition formulation, replacing temperature with enthalpy as the state variable. The model is presented in a fractional flow form that is advantageous for numerical solution techniques.

Fractures are modeled as two-dimensional features within the three-dimensional porous medium, and we propose a mixed-dimensional extension of the compositional multiphase flow model to capture the intricate dynamics of high-enthalpy fractured geothermal reservoirs. This model enables robust simulation of fluid flow, heat transfer, and phase separation, while also accounting for interactions between processes in the fractures and the surrounding porous medium.

In terms of numerical methodology, our work introduces two significant contributions:

- We have developed a mixed-dimensional hybrid upwinding technique for compositional flow, which enhances the numerical stability of gravitational segregation in the presence of sharp density gradients.
- We have developed an efficient interpolation scheme for H₂O–NaCl brine correlations in pressure-enthalpy-composition (PHZ) space, allowing complex thermodynamic properties to be integrated into the simulation with both accuracy and efficiency.

Several simulations of complex flow dynamics, particularly in fractured geothermal reservoirs with challenging fracture network geometries, are presented.

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Water & Porous Media Focused Abstracts:

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References:

MS09 / 475

Pore-scale modeling of reactive transport in complex porous media

Author: Sergi Molins¹

Co-author: David Trebotich

¹ *Lawrence Berkeley National Laboratory*

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Porous media are characterized by their physical and mineralogical heterogeneity at spatial scales from nanometers to meters. Fluid flow and solute transport may have characteristic scales that span orders of magnitude in complex porous media. As a result, relatively large gradients in geochemical conditions may exist in regions in close proximity. Pore scale models have been successfully used to simulate flow and reactive transport in natural and engineered media but are still challenged by the size of the domain and the complexity of the pore structures they can consider or the ability to capture processes with different characteristic scales. Here we develop a pore scale model to quantify the relationship between porous media heterogeneity and the development of these geochemical gradients which ultimately determine the effective reaction rates in subsurface applications. Advantages of our approach include the ability to construct complex porous geometries, and to perform high resolution simulations on HPC platforms that make use of accelerators. We demonstrate the use of the model in quantifying effective rates of weathering and mineralization reactions in complex porous media.

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477

Effects of Microplastics on Thermal Conductivity, Surface Albedo, and Temperature in Sandy Soils

Author: Milad Aminzadeh¹

Co-authors: Tanmay Kokate²; Nima Shokri¹

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Soils, unfortunately, act as significant reservoirs for microplastics (MPs), which alter their intrinsic properties and influence soil physical, biological, and hydrological processes (Jannesarahmadi et al., 2023). This study investigates the impact of MPs with varying characteristics on soil temperature dynamics through laboratory experiments. We measured changes in soil thermal conductivity and surface albedo in the presence of polyethylene (PE) and polyvinyl chloride (PVC) particles at different concentrations. Our results show that MPs, particularly PVC, reduce the effective thermal conductivity of sand by up to 38%. Additionally, surface deposition of MPs increased albedo by 28% and 77% with 5% PVC and PE, respectively. These changes affected soil temperature dynamics, as evidenced by altered evaporative fluxes and subsurface temperature profiles measured in drying sand columns. Our results extend the understanding required to describe the effects of MPs on soil thermal behavior.

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References:

Jannesarahmadi, S.; Aminzadeh, M., Raga, R., Shokri, N. (2023), Effects of microplastics on evaporation dynamics in porous media, *Chemosphere*, 311, 137023, <https://doi.org/10.1016/j.chemosphere.2022.137023>

480

Experimental evaluation of pore size, mineral composition, and transport regime controls on mineral precipitation in porous media

Author: CHIMA UKAOMAH¹

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Reservoir changes in bulk porosity and permeability induced by mineral precipitation can reduce the efficiency of energy production and CO₂ storage operations. The efficiency of these operations will be greatly improved if precipitation-induced changes to the bulk reservoir porosity and permeability can be accurately predicted via models that factor the influence of measurable variables like the initial PSD, transport regime, and mineralogical composition of the rock pore surfaces. This study evaluates the influence of PSD and transport regime on precipitation-induced changes to PSD and permeability in geologic media through micro-computed tomography (μ CT) and small angle neutron scattering (SANS) analysis of microporous quartz-rich Berea sandstone and calcite-rich Indiana limestone rock samples was conducted before and after calcite precipitation was induced under conditions representing high Péclet number and low Péclet number transport regimes, while subjecting the samples to typical reservoir temperature and pressure conditions. Post-experiment, a reduction in bulk porosity and permeability was observed in both samples after precipitation was induced at high and low Péclet number conditions. The pore size distribution (PSD) obtained from μ CT analysis revealed that at the micro-scale, this resulted in the samples being characterized by a right-skewed shift in PSD after precipitation was induced. However, under low Péclet number conditions, the rock samples were observed to have a greater decrease in bulk porosity due to the filling of large and small microscale pores. Results from μ CT analysis revealed that when precipitation is induced under high Péclet number conditions, a greater decrease in bulk porosity and permeability will be observed in rock samples with a high pore connectivity. Nanoscale pore structure results from SANS analysis of microporous calcite-rich Indiana limestone samples also reveal that nanoscale pore volume reductions due to a precipitation-induced clogging of large to small nanopores are greater when the transport regime is advection-limited. Overall, such nanoscale to microscale insights on the coupled PSD and transport dependence of precipitation-induced permeability reduction is crucial to accurately modelling reservoir porosity and permeability evolution during engineering applications such as CO₂ storage, hydrocarbon recovery, and geothermal energy production.

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Water & Porous Media Focused Abstracts:**References:**

MS06-A / 482

Quantifying the Effect of Pore-size Dependent Wettability on Relative Permeabilities using Lattice Boltzmann Simulation

Author: Siqin Yu¹

Co-authors: Mohamed Mehana ; Eric Guiltinan ²; Timothy Germann ²; Michael Gross ²; Qinjun Kang ²

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Relative permeability is a crucial two-phase property in porous media that can be significantly impacted by wettability conditions. While traditional research has predominantly examined homogeneous wettability, this work explores the less studied pore-size dependent (PSD) wettability, featured by a pore-size dependent wettability distribution. Leveraging high-fidelity Lattice Boltzmann simulations on CT-scanned porous samples, we demonstrate how PSD wettability would impact relative permeability at the pore scale. Our findings reveal that the deviation of relative permeability from the homogeneous wettability induced by PSD wettability can be 5% to 20%. The deviation of relative permeability curves increases as the spanning range of the contact angle increases. We also find that this impact is less pronounced as the capillary number increases. By adopting a pore-size-dependent contact angle relationship, our approach provides a more accurate and nuanced understanding of how PSD wettability would impact two-phase flow. These findings discovered at the pore scale may also provide valuable insights on relative permeability at the core to reservoir scales.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

MS07 / 483

A proposal to model non-uniform mixing of polymers in flows of shear-thinning polymers in porous media during enhanced oil recovery by polymer flooding

Author: Prabir Daripa¹

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In modeling flows of shear-thinning polymers in porous media, it is usually assumed that the polymer is uniformly mixed in the aqueous phase in space and time. However, this is rarely the case after an initial period of flow through the porous media. Even though there does not exist any theory of how the non-uniformity in mixing develops in time and space, we propose a modeling approach to include initial non-uniform distribution of polymer in the aqueous phase. We perform numerical simulations of polymer flooding using a hybrid method [1,2] to evaluate the effect of such non-uniform mixing of shear-thinning polymer [3] on the porous media flow and oil recovery. We will present results for several levels of non-uniform mixing for two polymers at multiple injection rates and initial polymer concentrations.

Publications Reference:

[1] Prabir Daripa and Sourav Dutta, Modeling and Simulation of Surfactant-Polymer Flooding using a New Hybrid Method, J. Comp. Phys., 335, pp. 249-282, 2017.

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Poster / 487

Correlative characterization of fluid flow and solute transport in disordered porous media via fast micro-computed tomography

Authors: Ronny Pini¹; Takeshi Kurotori¹

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The study of fluid-flow and solute transport in natural porous media has applications across diverse geological environments, such as soils for contaminant remediation and rocks for subsurface gas (CO₂ or H₂ storage). Transport processes drive chemical reactions in fluids; however, the inherent disorder of natural porous media introduces heterogeneities in physico-chemical properties across

a wide range of length scales. This disorder results in heterogeneous velocity fields, which in turn produce complex and difficult-to-predict solute concentration distributions, leading to the so-called “non-Fickian” behavior.

Solute transport in rocks is often studied using 4D imaging techniques such as X-ray and neutron-based computed tomography. While these methods enhance our understanding of non-Fickian transport [1], their limited spatial resolution (>1 mm) precludes direct observations at the pore-scale where the mixing processes originates. The development of fast X-ray CT imaging allows direct visualization of pore-scale processes at much finer spatial and temporal resolution (approx. few μm and 10 sec). However, quantitative analysis of the imagery obtained by these approaches is still lagging, with significant potential for optimization in geological applications.

Here, we analyzed a comprehensive 4D dataset obtained via fast micro-computed tomography from tracer tests conducted in two sintered glass beadpacks (6 mm diameter, 20 mm length) with irregular grain and pore structures [2,3]. Tracer experiments were performed at two Péclet numbers ($Pe = 2.7$ and 5.4), with scans acquired over a $6\text{ mm} \times 5\text{ mm}$ window at spatial and temporal resolutions of $13\text{ }\mu\text{m}$ and 15 seconds, respectively. We found that the pore space must be clustered into larger sub-volume elements—at least 700 times the voxel size in this case—to enable reliable quantification of flow and transport properties. The dataset was rigorously evaluated using concentration profiles associated with each clustered pore-volume element (PVE) to produce arrival-time maps (as proxy for flow heterogeneity) and mixing maps (as proxy for transport heterogeneity). While slice-averaged properties could be well predicted by a simple transport model (the Advection Dispersion Equation, ADE), significant variability was observed at individual PVE locations. This variability became more pronounced at higher Pe primarily due to the emergence of flow channeling. Our findings demonstrate that fluid flow—primarily driven by pore connectivity and pore-size heterogeneity—does not necessarily dictate solute transport dynamics. The distinct features of the arrival-time maps and the mixing maps indicate that both data-sets are necessary to fully capture the solute transport process. As such, these results highlight the benefits of further developing correlative characterisation techniques in the study of solute transport in porous media.

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MS26 / 489

Direct observations of solute dispersion in rocks with distinct degree of sub-micron porosity

Author: Takeshi Kurotori¹

Co-authors: Christopher Zahasky²; Sally Benson³; Ronny Pini¹

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The transport of chemical species in subsurface rocks is influenced by their structural heterogeneity, resulting in a wide range of local solute concentrations. In the context of CO₂ storage, understanding chemical transport is crucial for processes such as the convective dissolution of CO₂-rich brine in saline aquifers and the precipitation or dissolution of CaCO₃ in carbonate reservoirs - processes driven by mixing between miscible fluids. To accurately quantify these spatial mixing behaviors, advanced methodologies are required for detailed characterization of both the rock's spatial heterogeneity and the resulting solute concentration distributions within the fluids.

In this study, we demonstrate the application of asynchronous multimodal imaging using X-ray computed tomography (XCT) and positron emission tomography (PET) to investigate passive tracer experiments in laboratory rock cores with varying degrees of subcore-scale heterogeneity and microporosity [1]. The four-dimensional concentration maps generated by PET reveal distinct signatures of the transport process, which we quantify using concentration probability density functions and fundamental measures of mixing and spreading. We observe that solute spreading strongly correlates with the degree of subcore-scale porosity heterogeneity measured by XCT. However, the extent of spreading is significantly moderated by the presence of sub-micron porosity, which enhances dilution and ultimately contributes to the so-called “anomalous transport” observed in breakthrough curves.

The PET imaging approach is capable of distinguishing between spreading and mixing in heterogeneous media. By complementing it with XCT, this distinctive behavior can be directly correlated to the strength and structure of subcore-scale heterogeneity. The proposed workflow bears important implications because classical breakthrough curve analysis cannot be used to unequivocally separate the effects of spreading and mixing. The dataset generated in this study [2] provides a foundation for developing realistic digital rock models and benchmarking transport simulations that incorporate rock property heterogeneity in a deterministic manner.

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- [1] Kurotori, T., Zahasky, C., Benson, S., and Pini, R. (2024). Direct observations of solute dispersion in rocks with distinct degree of sub-micron porosity. Authorea. <https://doi.org/10.22541/au.172426895.50891936/v1>.
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MS03 / 490

Particle transport in propagating hydro-fracture

Author: YUJING DU¹

Co-authors: Thomas Cochard ²; Ilya Svetlizky ³; Congcong Yuan ⁴; Yiqiao Song ²; Lizhi Xiao ⁵; David A. Weitz ⁶

¹ *The University of Tulsa*

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Hydraulic fracturing is a technique that involves injecting fluids into rock formations at high pressure to create cracks or hydro-fractures. While hydro-fracture can occur naturally during seismic events, hydraulic fracturing is a human-engineered process used to increase the permeability of low-permeability rock formations. This technique is widely applied in engineering applications such as oil and gas extraction, carbon sequestration, and geothermal energy production. Hydro-fracture tends to close due to the compressive stress from the surrounding rocks when fluid pressure decreases, which is unfavorable in applications, where maintaining open fractures is essential. To prevent fracture closure, particles known as proppants, are added to the fracturing fluids and co-injected into the hydro-fracture. Therefore, the effectiveness heavily depends on the efficient delivery to the desirable locations within the hydro-fracture. While the behavior of particle-laden fluids has been extensively studied, there is much less understanding of the particle transport dynamics within a hydro-fracture due to the complex interplay between fracture geometry, particle properties, and fluid flow characteristics within hydro-fracture. Exploring the impacts of various forces and factors that influence particle transport in hydro-fracture is crucial for accurately predicting the performance of proppants in fracture operations.

In the experiment, we introduce particles into fracturing fluids and induce a penny-shaped fracture in a PMMA cylindrical sample by injecting the fracturing fluids at high pressures. We visualize the particle transport process during hydrofracturing by high-speed imaging. The PMMA cylindrical sample is created using the stereolithography 3D printing technique, which uses ultraviolet laser light to cure liquid photopolymer monomers into a solid form. In the experiment, the sample is positioned horizontally, and the vertical hole is prefilled with a particle-fluid mixture. Water is injected into the vertical hole at a constant rate using a high-pressure syringe pump, gradually increasing the pressure to initiate a crack in the sample. The process is recorded from the bottom of the sample using a high-speed camera, enabling the identification and tracking of particles in the captured videos.

We demonstrate how fluid flow characteristics and fracture geometry jointly affect particle transport in hydro-fractures. Our findings reveal that particles closely follow the fracturing fluid flow until they are trapped by geometric size exclusion near the fracture tip, where the narrowing aperture prevents larger particles from passing through in water-driven hydro-fractures. Flow instability, characterized by vortex formation, further disrupts particle transport by entraining particles into swirls, altering their trajectories. In contrast, with viscous fluids such as glycerol-water mixtures, particle lag is negligible. Increased viscosity widens the fracture aperture and suppresses vortex formation, allowing larger particles to reach the fluid front with reduced disturbance. This work provides essential insights into the mechanisms governing particle transport in hydro-fracture, revealing how fluid viscosity, flow characteristics, and fracture geometry influence particle transport dynamics, which is important for optimizing proppant placement in hydraulic fracturing operations.

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MS19 / 491

Fabrication of electrospun micro porous layers for enhanced green hydrogen production**Author:** Sergio Diaz¹**Co-authors:** Kui Li ¹; Wipula Liyanage ¹; Jacob Spendelow ¹; Siddharth Komini Babu ¹¹ *Los Alamos National Laboratory***Corresponding Authors:** sergio.diaz@lanl.gov, kuili@lanl.gov, wipula@lanl.gov, skb@lanl.gov, spendelow@lanl.gov

Proton exchange membrane water electrolyzers (PEMWEs) face performance limitations due to the poor interfacial contact between the catalyst layer and the porous transport layers (PTLs). This issue reduces catalyst utilization and increases contact resistance, leading to non-uniform exposure to applied voltages or currents. Such non-uniformities not only lower efficiency but also accelerate catalyst degradation. While increasing anode catalyst loadings can partially address these challenges, doing so conflicts with efforts to minimize the use of precious metals to reduce system costs. Additionally, the poor in-plane conductivity of anode catalysts further aggravates these limitations. Micro-porous layers (MPLs) have emerged as a promising solution to these interfacial challenges. By providing high surface area and small pore sizes, MPLs can significantly improve contact with the catalyst layer, enhancing catalyst utilization and reducing contact resistance. Furthermore, the hierarchical structure of MPLs facilitates more effective oxygen removal and improves water transport to the anode catalyst layer, addressing mass transport limitations and supporting stable operation. In this study, titanium-based MPLs were fabricated through electrospinning, using a titanium precursor and a carrier polymer. Electrospinning was chosen due to its superior control over fiber morphology and uniformity. The resulting electrospun fibers were calcined to produce TiO₂ fibers, forming the MPL structure. To ensure robust integration, the MPL was incorporated into a commercial felt-based PTL substrate using hot-pressing and sintering techniques. This approach aimed to optimize the physical and electrical connections between the MPL and the PTL substrate, enhancing overall performance.

Electrochemical performance of the MPL-PTL assemblies was evaluated through polarization curves, electrochemical impedance spectroscopy (EIS), and cyclic voltammetry. These analyses provided insights into the improvements in catalyst utilization, contact resistance, and mass transport properties achieved by integrating MPLs. Surface characterization of the MPL and catalyst layer was performed before and after electrolyzer testing using scanning electron microscopy (SEM) and laser profilometry. These techniques revealed structural and morphological changes, further highlighting the effectiveness of MPLs in improving interfacial properties and durability. This study demonstrates that titanium-based MPLs offer a viable pathway to address interfacial limitations in PEMWEs. By improving integration and enhancing transport properties, these MPLs have the potential to reduce catalyst loading requirements while maintaining or even improving performance, thereby contributing to the development of more cost-effective and durable electrolyzer systems.

Acknowledgements

This research is supported by the U.S. Department of Energy (DOE) Hydrogen and Fuel Cell Technologies Office through the Hydrogen from Next-generation Electrolyzers of Water (H2NEW) consortium. Program manager Dave Peterson and Mackenzie Hubert.

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Student Awards:**Water & Porous Media Focused Abstracts:**

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492

Microfluidic Investigation of Static and Dynamic Hydrogen-Methane Mixtures Relevant to UHS at 850 psi and 20-50 °C**Authors:** John Andresen¹; Nikolaos Diamantakis¹; Omid Shahrokhi¹¹ Heriot-Watt University**Corresponding Authors:** j.andresen@hw.ac.uk, nd2025@hw.ac.uk, o.shahrokhi@hw.ac.uk

Underground Hydrogen Storage (UHS) has gained significant attention recently as an efficient means of storing green energy. The unique challenges of hydrogen, such as its low ambient density (Muhammed et al., 2022) and its high flammability with atmospheric oxygen across a wide concentration range (Dagdougui et al., 2018) necessitates the use of deep geological formations. Among these, depleted gas reservoirs stand out due to their proven containment security, reduced losses compared to aquifers and depleted oil reservoirs, and existing infrastructure that can be repurposed for hydrogen storage (Muhammed et al., 2022; Al-Shafi et al., 2023; Zivar et al., 2021). The residual native natural gas in depleted gas reservoirs, minimizes the need for cushion gas, (Carden and Paterson, 1979; Bragg and Shallenberger, 1976; Ahmed, 2010; Tarkowski et al., 2021) essential for pressurization and hydrogen withdrawal (Carden and Paterson, 1979).

This study investigates the influence of methane, as a proxy for natural gas, on UHS through microfluidic experiments simulating drainage and subsequent imbibition processes at conditions representative to shallow reservoirs. More specifically, the potential effect of the dynamic mixing between hydrogen and methane is investigated. Hydrogen and methane reflect a significant enthalpy of mixing, which increases with pressure, resulting in a reduced temperature of the mixture, thereby changing the thermodynamic properties of the resident fluids (Lewis et al., 1977; Xue et al., 2018). These temperature changes, significant at typical UHS pressures, may impact the overall UHS process, including storage capacity and withdrawal efficiency.

The experiments are conducted at conditions representative for shallow gas reservoirs i.e. 850 psi and 20-50 °C. Mixtures of 50 mol% H₂ –50 mol% CH₄, 70 mol% H₂ –30 mol% CH₄ are examined alongside pure H₂ and pure CH₄ injections. Moreover, the influence of dynamic mixing is investigated with the use of a dual port injection in which H₂ and CH₄ are injected simultaneously in a controlled way into the glass chip. The obtained images are initially processed with ImageJ followed by filtering and phase segmentation using Avizo Pro. This way, the gas phase storage capacity and withdrawal efficiency are calculated after each drainage and imbibition cycle, respectively. This is one of the first studies to evaluate the effect of dynamic mixing of hydrogen and methane with respect to UHS processes, to the best of the authors knowledge.

The analysis is ongoing, but preliminary results (Fig.1) reflect some differences in terms of the storage capacity and connectivity of gas ganglia in between the dynamic and static mixture injection cases, which are important for the understanding and optimization of UHS operations.

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MS15 / 493

Estimating Capillary Pressure Using Wasserstein Generative Adversarial Network With Gradient Penalty

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Capillary pressure plays a crucial role in multiphase transport and has applications in carbon dioxide sequestration and underground hydrogen storage. Characterizing it is challenging when rock samples are unavailable; thus, it is often estimated using the J function, but the scaled results are scattered. This presentation discusses a new approach for estimating capillary pressure using the Wasserstein Generative Adversarial Network with Gradient Penalty (WGAN-GP) to capture the complex relationships between capillary pressure, pore structure, permeability, and porosity. First, the study used Density-Based Spatial Clustering of Applications with Noise (DBSCAN) to cluster 118 rock samples recovered from depths ranging from 161 to 16,678 ft below the surface. Next, it converted their capillary pressure, permeability, and porosity measurements into images by introducing the concept of a constrained capillary pressure image. Then, it augmented the constrained images to increase their number to 1,166. Later, it designed a conditional WGAN-GP, with its hyperparameters tuned by analyzing the quality of generated images and loss values. The images generated in the best scenario showed no mode collapse; thus, they were converted back into capillary pressure measurements. The capillary pressures generated in the best scenario exhibit key characteristics of tight gas sandstones, such as partial percolation and nonzero entry pressure. The results are interesting and have applications in characterizing capillary pressure far from the wellbore.

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MS06-B / 497

Phase Nucleation in Pore Structures

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Phase nucleation on substrates with different geometries arises in many important industrial processes such as condensation, crystal growth, and desalination [1]. The nucleation behavior on planar or spherical surfaces has been accurately elucidated [2-3]. However, on the surfaces with complex geometries, the dependence of the energy barrier for forming a critical nucleus on the geometry and the wettability remain marginally explored. Herein, we propose a theoretical model to delineate the nucleation behavior on a generalized pore structure [4] with varying opening angles and contact angles. The proposed model can predict the volume of the critical nucleus formed within the

designed pore structure with an arbitrary opening angle and contact angle. Therefore, by spontaneously changing the opening angles and contact angles, the nucleation behavior on the pore-shaped substrate can be precisely manipulated. We also investigate the influence of the line tension effect on the nucleation behavior. Our findings provide an essential guideline for precise manipulation of nucleation behavior in designed pore structures to support potential applications for controlling self-assembled systems such as colloidal particles, block copolymers, and lipid nanoparticles.

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MS21 / 498

On the relation between the streamline- and volume-integrated tortuosity

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Tortuosity is one of the fundamental effective parameters describing hydrodynamic properties of porous media. However, the fact it can be defined in several different ways, e.g. via the length of the streamlines [1] or as a statistic of the pore-scale velocity field [2], may cause inconsistency between the results. For example, the equivalence between the weighted streamline-based tortuosity and easier to calculate volume-integrated tortuosity was analytically proven by Duda and others [2] for Stokes flows, with the latter being larger than the former when inertial effects show up. In the present work we study the sources of this inequality. In particular, we investigate the contributions to the tortuosity from the recirculation zones and the percolating part of the flow separately. We do so in terms of the volume of the recirculation zones and the kinetic energy/momentum contained therein, as well as the viscous momentum transfer from the percolating to the recirculation zones. We relate the changes of those quantities to the known regimes of inertial flows [3]. Our results explain the observations on the deviation from each other of the values of variously defined tortuosities, presented in previous works. They deepen the understanding of the pore-scale mechanisms of the onset of inertial effects in porous media and can serve as the theoretical baseline for the formulation of reduced models of inertial transport therein.

The picture shows the percolating volume of the flow through a periodic array of spheres for low (left) and high (right) Reynolds number. The flow is driven by a body force aligned with the x-direction.

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¹ Srisutthiyakorn, Nattavadee & Mavko, Gerald. (2017). What is the role of tortuosity in the Kozeny-Carman equation?. Interpretation. 5. SB57-SB67. 10.1190/INT-2016-0080.1., ² Duda, A. & Koza, Zbigniew & Matyka, Maciej. (2011). Hydraulic tortuosity in arbitrary porous media flow. Physical review. E, Statistical, nonlinear, and soft matter physics. 84. 036319. 10.1103/PhysRevE.84.036319. , [3] AGNAOU, Mehrez & Lasseux, Didier & Ahmadi-Sénichault, Azita. (2017). Origin of the inertial deviation from Darcy's law: An investigation from a microscopic flow analysis on two-dimensional model structures. Physical Review E. 96. 10.1103/PhysRevE.96.043105.

Poster / 499**Total Cost of Dissipative Transport in Poriferan Aquiferous Systems****Author:** Emile Kraus¹¹ *University of Pennsylvania***Corresponding Author:** emkraus@sas.upenn.edu

Aquatic sponge tissue is the quintessential living, porous, viscoelastic solid. These animals grow in a myriad of forms, intuitively to maximize flow through their unidirectional water and particulate transport system, or aquiferous system, however the data remain equivocal. Several studies have quantified the dissipative loss from hydraulic transport while ignoring friction from particle-tissue and particle-water interactions. Here, the conceptual power behind the unique physiology of a sponge is used as leverage. Since dissolved particle transport through their bodies is unidirectional, the operation of a living sponge is a prescient example of a coupled irreversible transport process. Onsager transport equations are presented, and meta-analyses reveal estimates of transport coefficients within a rigorous non-equilibrium thermodynamic framework. Sponge tissue is idealized as a complex network of parallel membranes following recent progress in Peusner network thermodynamics, and preliminary lattice Boltzmann simulations are presented.

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500

Effect of Skin on the CO₂ Injection Conditions in a Heterogeneous Reservoir

Author: Lorena Cardoso Batista Aum¹

Co-authors: Pedro Tupã Pandava Aum¹; Thiago Henrique da Silva Barbosa¹; Claudio Regis dos Santos Lucas¹; José Jadsom Sampaio de Figueiredo¹

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The near-wellbore region plays a crucial role in determining production and injection conditions, directly impacting operational efficiency. Skin, as a dimensionless parameter representing wellbore damage or stimulation, critically alters petrophysical properties and thus injectivity. The injection of reactive fluids, such as supercritical CO₂, poses additional challenges due to its capability to modify rock-fluid interactions, particularly within heterogeneous reservoirs like those found in the Brazilian Pre-Salt formations. Understanding the dynamic influence of skin in such conditions is vital for optimizing CO₂ storage and enhancing injection efficiency.

This study investigates the impact of varying skin conditions on CO₂ injectivity and storage capacity over a 25-year simulation period. A heterogeneous reservoir model was used, incorporating realistic properties from the Brazilian Pre-Salt region. Skin factors ranged from -5, indicating well stimulation, to +5, reflecting severe damage. The simulations evaluated the correlation between skin and reservoir

pressure, assessing their combined effects on fluid injectivity and storage potential.

The results highlight that positive skin values (damage) significantly impede injectivity, reducing the total volume of CO₂ that can be stored in time. The associated pressure buildup in injection wells can exceed operational thresholds, posing risks to equipment integrity and overall project feasibility. In contrast, negative skin values (stimulation) improve fluid acceptance, demonstrating increased injectivity and storage efficiency. This finding underscores the importance of mitigating wellbore damage and employing stimulation techniques to achieve optimal performance in CO₂ storage projects.

These results can assist with managing CO₂ injection operations in heterogeneous reservoirs. By addressing skin-related challenges, operators can better control injection pressures and maximize storage efficiency, contributing to the global effort to reduce greenhouse gas emissions through effective carbon sequestration.

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501

Modeling multiphase Flow in Thin Absorbent Swelling Porous Materials

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Wicking in thin media plays a crucial role in liquid absorption across a wide range of applications, including wipes, diapers, medical devices, sportswear, filtration, batteries, and oil spill cleanup. This chapter introduces a sophisticated mathematical modeling framework to analyze liquid absorption and solid deformation during unsaturated two-phase flow in thin, swelling porous media under isothermal conditions. By applying a volume averaging approach, three-dimensional point-wise mass balance equations are transformed into quasi two-dimensional averaged equations. These macroscopic mass balance equations are then coupled with a series of constitutive relationships. A closure model is proposed to describe the inter-layer mass exchange of liquid, while a deformation model, based on nonlinear elasticity theory, is used to account for layer compression. The models presented significantly enhance computational efficiency, allowing for faster, cost-effective simulations of the absorbency process in partially-saturated porous media, such as fiber and hydro-gel composites. This framework deepens our understanding of wicking in thin media, facilitating its optimization across diverse industrial and environmental applications.

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MS26 / 502

Preliminary findings from the GFV experiment: Investigating the role of multiscale geological heterogeneity on plume migration and trapping

Author: Sally Benson¹

Co-authors: Achyut Mishra²; Ahmad Mortazavi³; Aman Raizada¹; Catherine Callas¹; Catherine Spurin¹; David Bason³; Julie Dickinson³; Louis Durlofsky¹; Max Watson⁴; Mitch Allison⁴; Oleg Volkov¹; Peter Cook³; Ralf Haese³; Richard Larson¹; Stephan Matthai³; Xin Ju¹

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In 2023 the GeoCquest project team joined forces with the CO2CRC in Australia to design and carry out the GeoCquest Field Validation (GFV) Experiment at the Otway International Test Centre. The goal of the experiment is to test and refine approaches for predicting plume migration and trapping in highly heterogeneous rocks using advanced multiscale characterization and simulation approaches, including: geomodeling with composite rock types; petrophysical characterization of directional and

rate-dependent relative permeability and capillary pressure functions; and high-resolution reservoir simulation. Between November 2024 and January 2025, 10,000 metric tons of supercritical fluid containing 80% CO₂ and 20% CH₄ is being injected into a 10-m thick interval at a depth of 1450 m in a highly heterogeneous sandstone in the Paaratte Formation of the Otway Basin. The plume is moving updip to intersect CRC-8, a passive purpose-built monitoring well where daily saturation measurements are being obtained with a high-resolution pulsed neutron logging instrument (PNL) over a period of 5-6 months. Plume saturation measurements are being made during both the injection and post-injection phases, to enable observations of plume migration followed by residual gas trapping. Solubility trapping will be measured by fluid sampling at the injection well in and above the injection zone after injection stops.

Continuous core was collected in both the injection well (CRC-3) and a newly drilled well (CRC-8), located 115 m updip of the injection well. A new high resolution (0.3m x 3.3 m x 3.3 m) geo-model has been developed based on a combination of well log, core, and seismic data, that includes 2 homogeneous and 4 composite rock types that are representative of the reservoir in this depth interval. Detailed petrophysical characterization of the cores includes continuous CT, minipermeameter measurements, routine core analysis, special core analysis for capillary pressure and relative permeability measurements in each of the major rock types, as well as a suite of cased-hole well logs.

Our presentation will provide an overview of preliminary results from the experiment, including CO₂ plume migration and saturations as measured by the PNL, injectivity and pressure buildup, and temperature measurements made using behind-casing fiber optic sensors. In addition, we will present comparisons of probabilistic predictions of plume migration and trapping using two modeling approaches: 1) full physics modeling using GEOS and 2) a machine learning model (CCSNet.ai). These pre-injection predictions provide a benchmark against which to compare actual plume migration and trapping. Together, work elements of the GFV experiment are designed to test, improve, and validate multiscale approaches for predicting the performance of geological storage in highly heterogeneous environments.

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504

Pore-scale Modelling of salt precipitation during CCS

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Carbon Capture and Storage (CCS) is considered a necessary technology for mitigating climate change, helping to keep temperature increases within the limits set by the Paris Agreement. In CCS,

CO₂ is captured from anthropogenic sources and is injected into deep saline aquifers, depleted oil and gas reservoirs or other geological traps. Deep saline aquifers play an important role as their capacity for safe storage of CO₂ is two orders of magnitude greater than depleted oil and gas reservoirs. Maintaining the injection of CO₂ into the subsurface is a critical part of determining the success of any CCS project; however, this is not always straightforward. Former studies show that injecting dry super-critical CO₂ in saline and hypersaline aquifers leads to dry-out and formation of salt precipitation in porous space. This can cause significant decrease in permeability, leading to potential loss of injectivity. Addressing this challenge requires developing a fundamental understanding and predictive capability for injectivity loss under various conditions, including thermodynamic (pressure and temperature), hydrodynamic (injection rate), and rock heterogeneity factors. Salt precipitation arises from coupled physical, chemical, and transport processes operating across multiple length and time scales, making it a complex multi-physics, multi-scale problem (Ott et al., 2012, 2014, 2015, 2021). In the present work, we develop a quasi-static, semi-dynamic pore-network model to elucidate salt-formation mechanisms at the pore scale under diverse conditions. Our model captures the interplay of capillary-driven flow (including capillary backflow), evaporation, and salt precipitation. Key features include:

1. Quasi-static (QS) two-phase pore-network modeling (extending Niasar et al., 2009).
2. Capillary-driven backflow implemented through cluster labeling.
3. Kelvin effect.
4. Irregular pore-network geometry (unstructured, randomly distributed) with triangular pore-throat cross-sections.
5. Advection-diffusion transport of vapor.
6. Hygroscopic effect of salt in the liquid phase via an additional potential term in the Kelvin equation.
7. Salt precipitation feedback on the pore-network geometry, influencing transport dynamics.

Existing pore-network models that consider evaporation (Maalal et al., 2021; Dashtian et al., 2018; Ahmed et al., 2020) typically incorporate features (1-3) and rely on idealized geometries (e.g., lattice networks) without considering how salt precipitation alters the transport behavior. In contrast, our model (4) adopts a more realistic pore-network structure, (5) captures the essential physics of evaporation, and (6-7) accounts for salt precipitation feedback on the system.

We demonstrate that our model reproduces the characteristic stages of evaporation in porous media observed in experiments. In particular, the initial high evaporation rate “Stage I” is followed by the “Stage II” falling-rate period in which the evaporation rate decreases significantly. We then examined the hypothesis, “Is a quasi-static PNM approach suitable for modeling salt precipitation?” Our results indicate that the purely advective time scale is approximately half that of the case with evaporation and salt precipitation, implying that advective flow proceeds faster than diffusive vapor transport. Hence, the quasi-static modeling assumption is justified for capturing the essential dynamics of evaporation and salt precipitation in porous media.

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Poster / 505

Numerical modeling of Complex Fluid injection for LNAPL displacement: Insights from 1D Column Experiments

Author: Dana Sapobekova¹

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Contamination of soils and aquifers by light non-aqueous phase liquids (LNAPLs) poses significant risks to environmental sustainability and public health. Conventional in-situ LNAPL remediation techniques often encounter high costs and limited efficiency challenges, leaving residual hydrocarbons trapped within soil pores. As an alternative, unconventional in-situ flushing using complex shear-thinning fluids —such as polymers, foam, emulsions, etc. —has emerged as a promising approach. These advanced fluids enhance contaminant recovery through their high viscosity and non-Newtonian shear-thinning properties, ensuring stable and uniform displacement within porous media.

This study, which investigates the performance and flow behavior of aqueous biopolymers in porous media through a series of one-dimensional (1D) sand-packed column experiments, provides a solid foundation for further numerical modeling efforts. The primary objective is to assess the potential and feasibility of using reservoir simulators for soil remediation in LNAPL-contaminated environments while exploring upscaling approaches to implement these techniques effectively at the field scale.

The model was developed using the Builder package in the CMG reservoir simulator, with numerical computations performed via the IMEX and STARS simulation packages. It employs the black oil model equations to describe a two-phase flow system, where the LNAPL is defined as the oil phase, and the polymer is represented within the aqueous solution.

One-dimensional (1D) column experiments served as the foundation for modeling bio-polymer injection. These experiments thoroughly assessed the polymer's recovery efficiency in displacing LNAPL (here diesel fuel) from unconsolidated, homogeneous porous media. The model was meticulously calibrated using experimental data by incorporating parameters such as porous media characteristics, dimensions, boundary conditions, and the properties of the injected and displaced fluids, ensuring accurate replication of the actual model conditions. A key challenge is adapting the simulator for the application in highly permeable porous media.

The modeling process revealed that the polymer behavior can be effectively adjusted by calibrating the injection fluid's endpoint mobility. This adjustment accurately represented the reduced mobility ratio observed during the experiments. As a result, the model demonstrated a stable displacement

front, with flow propagation as a function of injected pore volumes (PV) closely matching the experimental data. Furthermore, the model achieved a high recovery yield, successfully replicating the experimental outcomes and validating its accuracy in simulating polymer-assisted remediation processes.

The two-phase flow model demonstrated great agreement with experimental observations, validating its accuracy in representing the real case. This confirms the model's reliability as a tool for simulating polymer-assisted remediation processes. These results led us to upscale the process that can be applied to field case problems.

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MS12 / 506

DETERMINATION OF DISPLACEMENT FIELDS USING DIGITAL IMAGE PROCESSING IN A TAILINGS DAM TEST MODEL UNDER INCREASING PORE WATER PRESSURE

Authors: Abraham Armah¹; Mehrdad Razavi¹; Richard Otoo¹

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Pore Water Pressure management within porous media, particularly in tailings dams, is essential for ensuring the structural integrity of mining operations and mitigating environmental risks. This research applies Digital Image Processing (DIP) techniques to determine displacement fields in a laboratory-scale tailings dam model under controlled conditions. The implications of this research extend beyond tailings dam safety. It contributes to the broader understanding of water's role in the mechanical behavior of porous media, which is crucial for various applications, including ground-water management, soil stability, and hydrological engineering.

The experimental setup involves a tailings dam model subjected to a gradual increase in pore water pressure to simulate failure conditions. High-resolution images are captured continuously throughout the process, and advanced DIP techniques are employed to analyze deformation patterns. The research quantifies displacements and highlights the evolution of deformation within the porous media under stress-induced conditions.

This study is novel in its integration of non-invasive DIP methods to detect early-stage deformation patterns that precede catastrophic failures, which are often missed by conventional monitoring techniques. This approach is particularly relevant in managing water pressure within porous media, addressing critical gaps in tailings dam monitoring practices.

Key findings reveal a strong correlation between pore water pressure increases and deformation trends, emphasizing the significant role of water dynamics within the dam's structure. Visualizing displacement fields provides a deeper understanding of how stress propagates through porous materials, enabling more accurate modeling and risk assessment of tailings dams. Additionally, the technique offers a cost-effective, scalable, and environmentally friendly alternative to traditional monitoring methods.

By advancing the technical competence of geotechnical engineering practices, this study supports

the development of safer and more sustainable approaches to managing porous media in water-sensitive environments.

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Soil redox dynamics mediated by interacting biological and physical processes during Managed Aquifer Recharge

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Managed aquifer recharge (MAR) strategies hold potential for improving groundwater quantity for crop irrigation, yet they also pose risks to groundwater quality. The introduction of exogenous water into the subsurface, whether by flooding or well injection, creates geochemical gradients in redox potential, pH, and major ion compositions. In turn, these gradients can induce dissolution reactions in the aquifer matrix that can mobilize geogenic contaminants with the percolating water. This work aims to elucidate the impact that MAR has on redox shifts in the vadose zone, understanding that this change is at the heart of both arsenic and uranium mobilization. We pose that redox potential transients arise from the interplay between imbibition of the vadose zone with oxygenated water, limitations in atmospheric gas exchange across the soil-water interface, and oxygen respiration by microbial activity. We simulate water infiltration dynamics and reactive transport of oxygen from a drywell at a typical wetting-draining schedule and compare the timescales of biological reaction to those of physical transport to explain the observed trends. Our results reveal that the magnitude and persistence of redox shifts are limited in spatial extent and duration, whereby microbial respiration and dilution work together to efficiently mitigate the geochemical changes caused during MAR. A deep understanding in the controls for biogeochemical shifts is imperative to provide substantive guidance on sustainable water management strategies and to reduce potential long-lasting impacts on contaminant mobilization.

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MS07 / 511

Intracellular "in silico microscopes" - fully 3D spatio-temporal virus replication model simulations

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Despite being small and simple structured in comparison to their victims, virus particles have the potential to harm severely and even kill highly developed species such as humans. To face upcoming virus pandemics, detailed quantitative biophysical understanding of intracellular virus replication mechanisms is crucial. Unveiling the relationship of form and function will allow to determine putative attack points relevant for the systematic development of direct antiviral agents (DAA) and potent vaccines. Biophysical investigations of spatio-temporal dynamics of intracellular virus replication so far are rare.

We are developing a framework to allow for fully spatio-temporally resolved virus replication dynamics simulations based on partial differential equation models (PDE) and evaluated with advanced numerical methods on large supercomputers. This study presents an advanced highly nonlinear model of the genome replication cycle of a specific RNA virus, the Hepatitis C virus (HCV). The diffusion-reaction model mimics the interplay of the major components of the viral RNA (VRNA) cycle, namely non structural viral proteins (NSP), VRNA and a generic host factor (energy supply etc.). Technically, we couple surface PDEs (sufPDEs) on the 3D embedded 2D Endoplasmatic Reticulum (ER) manifold with PDEs in the 3D membranous web (MW) and cytosol volume. (The MWs are the replication factories growing on the ER induced by NSPs.) The sufPDE/PDE model is evaluated at realistic reconstructed cell geometries which are based on experimental data. The simulations couple the effects of NSPs which are restricted to the ER surface with effects appearing in the volume. The volume effects include the host factor supply from the cytosol and the MW dynamics. Special emphasis is put to the exchange of components between ER surface, MWs and cytosol volume. As the vRNA spatial properties are not fully understood so far in experiment, the model allows for vRNA both restricted to the ER and moving in the cytosol. The visualization of the simulation resembles a look into some sort of fully 3D resolved "in silico microscopes" to mirror and complement in vitro /in vivo experiments for the intracellular VRNA cycle dynamics. The output data are quantitatively consistent with experimental data and provoke advanced experimental studies to validate the model.

Country:

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

MS25 / 512

Geochemical Modelling CO₂ Mineralisation in Peridotite Formations, History Matching of a Pilot Test

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Efficient implementation of CO₂ mineralization can be a fast and safe method for the long-term disposal of anthropogenic CO₂. However, quantifying mineralized CO₂ can be a challenge in assessing CO₂ mineralization projects. Modelling can facilitate the long-term and large-scale assessment of mineralisation if a reliable model can be developed. Herein, a series of history-matching exercises was executed to calibrate the reaction kinetics behind CO₂ mineralization in fractured peridotite, using the results of a successful pilot test carried out in the peridotite of the Samail ophiolite in Oman. The pilot test, known as the Chalk project, was conducted in an inject-soak-retrieve mode. A fully coupled thermo-hydro-chemical reservoir model was developed to history match the pilot test using well-logging, core data, and well-testing analyses. Two realizations were constructed to investigate the role of grid size (coarse and fine grid size) in the history matching of reaction kinetics behind CO₂ mineralization. Additionally, two cases for the primary minerals of the host formation were considered: (i) Mg-rich olivine and (ii) serpentinized olivine.

For history-matching, the tracer concentration profile was matched as the baseline where no reaction takes place. Then, the reaction rate and surface area of primary and secondary minerals are tuned to reproduce the field observation. CMG-GEM package was used to perform the coupled simulations. The reaction rates of lizardite and pyroxene minerals were increased to enhance the dissolution, which helped match pH of the produced water. Also, dolomite and calcite were identified as the main carbonate minerals controlling the CO₂ mineralisation as they could match the trends of Ca and Mg, where the reaction rate and activation energy of precipitation for these two minerals were increased in the model. The dominance of dolomite and calcite in the modelling results matches field observations that reveal calcite and dolomite as the main carbonate minerals in the shallow subsurface (<200 m depth).

Also, overly coarse grids ease the progress of numerical simulation as the mixing of resident and injected fluid is better controlled in large grid volumes; however, large grid blocks fail to differentiate regions of the reservoir dominantly under dissolution or precipitation. Furthermore, using different primary minerals impacts the numerical stability of the reservoir model as well as the reaction kinetics. Serpentinized minerals such as lizardite could adversely affect numerical stability due to high reactivity.

From the various history-matching cases, it was concluded that the area of dissolution is very localized around the injection well, whereas precipitation takes place variably depending on whether it is calcium or magnesium-rich carbonates. Therefore, the gridding scheme of a reservoir model should differentiate the areas with predominant precipitation and dissolution. Additionally, the history-matched model was used for a long-term assessment of CO₂ mineralization in peridotite formations, where it demonstrated promising longevity for dissolution and precipitation projects. This work puts forward a robust methodology for modelling CO₂ mineralization in fractured formations. This work also demonstrates that using batch-based reaction kinetics may require further tuning for reservoir conditions, where dynamic dissolution and precipitation processes are in play.

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Water & Porous Media Focused Abstracts:

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References:

MS09 / 513

3D modeling of Ostwald ripening in multi-component carbon storage**Authors:** Jacques Franc¹; Christophe Blondeau²; patrice creux³¹ Université de Pau Pays d'Adour (UPPA) / Laboratoire des Fluides Complexes et de leurs Réservoirs (LFCR)² TotalEnergies³ CNRS/TOTAL/UNIV PAU & PAYS ADOUR/E2S, Laboratoire des Fluides Complexes et leurs Réservoirs IPRA, UMR5150, 64000 Pau, France.**Corresponding Authors:** patrice.creux@univ-pau.fr, christophe.blondeau@totalenergies.com, jacques.franc@univ-pau.fr

The geologic carbon sequestration and storage has been marked as one of the solution to remediate Global Warming. Structural and capillary trapping, residual trapping, solubility trapping and mineral trapping have been selected as important trapping processes to secure storage over time.

The stability of trapped CO_2 in geological reservoir is then a key factor in feasibility assessments and storage capacity predictions. Recently, many studies grew interest in Ostwald ripening during storage as a potential mechanism leading to bubble coalescence and hence potential instabilities.

Pore Network Modeling (PNM) is used here as a tool to enable simulation over larger networks. Its modeling of CO_2 ganglia is based on work from [Mehmani and Xu, 2022], capturing breakthrough, snap-off and drainage/re-imbibition events on multiple ganglia. It uses classical compositional transport in the brine-rich phase. The gas-rich phase is composed of multiple ganglia that served as boundary condition and are sequentially updated with respect to composition in their neighboring pores. After convergence, the gas distribution inside the ganglia is decided upon a stability test. It offers a modeling solution for different mechanisms, rock heterogeneities and conditions. It is also usually used as a first step for upscaling from pore to core scale, using statistically equivalent initial conditions and validating in the sense of distribution.

Complete 3D dynamics of ganglia are explored in different pore and throat radii's heterogeneities. Adjunction of an inert gas with a lower or no solubility in brine (e.g N_2) is also explored as a way of altering equilibrium state and hence ripening.

In the future similar modeling effort can be conducted to explore ripening occurring during H_2 storage. Its beneficial effects in re-mobilizing gas in order to produce it can be asserted under different storage conditions and production conditions.

Country:

France

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

Yashar Mehmani and Ke Xu. Capillary equilibration of trapped ganglia in porous media: A pore-network modeling approach. *Advances in Water Resources*, 166:104223, 2022.

MS18 / 515

Microbial safety of a variable flow-regime of Dutch drinking water production from groundwater wells

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Groundwater is the most important source of drinking water in many regions of the world. Farm animal manure, and wastewater from leaking sewers and septic tanks may contaminate groundwater. Soil acts as a natural filter (1), and therefore groundwater can be protected from contamination with pathogens by adequate setback distances (protection zones) between contamination sources and the groundwater well system (2).

According to the Dutch drinking water legislation, Dutch drinking water production companies are obligated to conduct a Quantitative Microbial Risk Analysis (QMRA) for drinking water production. The Guideline Analysis Microbiological Safety for Drinking Water provides information on how to conduct a QMRA for drinking water from surface water and groundwater (3). The guideline document is developed in cooperation with the environmental inspectorate and the drinking water companies.

The currently used QMRA model (4) is based on steady-state flow where mechanical filtering of pathogens occurs through a combination of low flow velocities and attaching/detaching probabilities, where in particular virus inactivation is primarily a time-dependent process. Increasing the residence time increases the probability of inactivating the virus, making the virus harmless.

In this talk, we will discuss the consequences of variable flow for the required setback distance. First, there is a dynamic change in balance between shortened travel time and dilution (from a greater volume being pumped). Secondly, a change in flow causes a temporal change in hydrostatic pressure. And finally, the frequency and magnitude of flow variations play a role.

With a higher demand for drinking water, and water scarcity (drought) and water surplus (intense rainfall) due to climate change, we argue that it is vital to include these dynamics into the QMRA calculations for drinking water safety.

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- 4) QMRAWell: QMRAWell | RIVM

MS02 / 516

Modelling and Model Validation Methods for Porous Media Solute Flow Problems

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In this talk I will outline combined experimental approach my group has taken to quantify porous media, such as soil, solute movement, such as plant nutrient P, movement using high temporal resolution techniques.

The reason for focusing on phosphorus is that it is an essential nutrient for crops. Precise spatiotemporal application of P fertilizer can improve plant P acquisition and reduce run-off losses of P. Optimizing application would benefit from understanding the dynamics of P release from a fertilizer pellet into bulk soil, which requires space- and time-resolved measurements of P concentration in soil solutions. In this study, we combined microdialysis and X-ray computed tomography to investigate P transport in soil. Microdialysis probes enabled repeated solute sampling from one location with minimal physical disturbance, and their small dimensions permitted spatially resolved monitoring. We observed a rapid initial release of P from the source, producing high dissolved P concentrations within the first 24 h, followed by a decrease in dissolved P over time compatible with adsorption onto soil particles. Soils with greater bulk density (i.e., reduced soil porosity) impeded the P pulse movement, which resulted in a less homogeneous distribution of total P in the soil column at the end of the experiment. The model fit to the data allow for the pinpoint identification of the processes involved in phosphorus behavior in soil in fine temporal resolution.

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MS26 / 517

Unraveling Salt Precipitation Mechanisms: Insights into Dominant Driving Forces

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Salt precipitation during underground CO₂ storage into saline aquifers poses a risk for injectivity impairment and presents a notable challenge for successful CO₂ storage initiatives. Laboratory studies indicate that salt precipitation is sensitive to capillary forces, but extending this to field-scale is non-trivial due to radial flow conditions, gravitational effects (e.g. gravity override), and geologic heterogeneity. The goal of this study is to use detailed 3D numerical simulation of salt precipitation to gain further insight into the controlling physical mechanisms in realistic storage formations. First, axi-symmetric homogeneous simulations are used to characterize salt precipitation under controlled conditions using non-dimensional parameters, e.g. capillary (Ca), Gravity (Gr) and Bond (Bo) numbers. Results confirm that smaller Ca generally encourages more capillary backflow and increased salt precipitation as expected. However, increasing Gr is found to impact the localization of salt deposits, i.e. gravity override causes salt deposits to form deeper and further into the storage reservoir. In addition, flow of CO₂ is redirected creating a feedback mechanism on local salt formation. These insights are used to understand salt precipitation observed in additional 3D simulations for heterogeneous systems. In layered systems, more salt is precipitated locally in higher permeability zones due to the lower Ca in those regions, causing flow to redirect into lower permeability zones that reduces the injectivity overall. For a random heterogeneity, the overall behavior holds with respect to Ca and Gr, but salt localization in a more complex permeability field exhibits an increased detrimental impact on injectivity than a simpler layered system. This study finds a strong coupling between salt precipitation and multiphase flow in 3D field-scale systems that can be characterized by capillary and gravity numbers. The ability to estimate salt precipitation from formation properties and anticipated injection rates is valuable for devising injection strategies for mitigating injectivity loss in industrial scale operations.

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References:

MS18 / 519

Mechanisms of foam transport and the role of injection parameters: A path to efficient remediation

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Soil and aquifer contamination by pollutants, including non-aqueous phase liquids (NAPLs) and per- and polyfluoroalkyl substances (PFAS), poses a severe threat to the environment and water re-

sources. Conventional remediation methods often achieve limited recovery efficiencies, underscoring the need for innovative and scalable technologies [1 - 2]. Aqueous foam, a fascinating two-phase fluid with a microstructure that profoundly influences flow behavior in porous media [3], offers a promising solution. However, maximizing remediation efficiency requires a deeper understanding of the complex dynamics of foam flow within subsurface environments, such as trapping and mobilization [4 - 6]. The main objective of this study is to provide new insights into the mechanisms governing foam flow in unconsolidated porous media as a precursor to the wider application of this technology.

The study introduces a novel experimental setup to investigate the flow of pre-generated foam composed of a Sodium Dodecyl Sulfate (SDS) and Cocamidopropyl Hydroxysultaine (CAHS) surfactant blend combined with nitrogen gas (N_2). Two injection protocols—fixed liquid flow and fixed gas flow—were employed to perform comprehensive foam quality (i.e., gas fractional flow) scans, assessing the influence of injection parameters on foam dynamics. The setup featured a 1D sandpack holder equipped with localized pressure and permittivity sensors, which allowed for the acquisition of pressure and saturation profiles along the system. High-resolution imaging enabled in-situ visualization of foam texture at the mesoscale (from pore to Darcy scale).

The results highlight the significant influence of gas compressibility on foam quality, emphasizing the importance of local pressure measurements for accurate assessment. Entrance and end effects were observed, underscoring the need to focus on internal sections of the porous medium for reliable interpretation of foam flow behavior. Foam quality scans revealed distinct low- and high-quality regimes, separated by a transition zone. Foam apparent viscosity showed a complex dependence on foam quality (f_g) and capillary number (N_{Ca}). Flowing and trapped foam fractions derived from local saturation measurements revealed a weak dependence on N_{Ca} at lower f_g (<0.85) and stronger at higher values. In-situ foam texture visualization captured dynamic variations in bubble size, highlighting the critical roles of lamellae division and bubble fragmentation in controlling foam mobility and flow uniformity.

This research advances foam-based remediation technologies by deepening our understanding of the mechanisms governing foam flow within porous media. By bridging laboratory-scale observations with practical applications, this study supports the establishment of aqueous foams as a viable tool for environmental remediation. Future work will focus on scaling these findings to heterogeneous field-like conditions, optimizing injection strategies, and expanding applications to diverse contaminants such as NAPLs and PFAS.

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France

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Student Awards:

Water & Porous Media Focused Abstracts:

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Model-based Reinforcement Learning for Optimal Control of Sub-surface Flow Systems

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Reinforcement Learning (RL) has recently gained traction as a promising tool for solving challenging control and optimization problems in porous media. In particular, subsurface reservoir management is a critical application domain, where optimal injection and production strategies can significantly enhance recovery while minimizing operational costs. However, purely model-free RL approaches often demand excessive computational budgets due to the large number of high-fidelity simulations needed during training.

In this work, we investigate model-based reinforcement learning (MBRL) as a more sample-efficient alternative for controlling two-phase flow in heterogeneous reservoirs. We focus on two state-of-the-art MBRL algorithms—Probabilistic Ensembles with Trajectory Sampling (PETS) and Model-Based Policy Optimization (MBPO)—which learn surrogate models of reservoir dynamics to either plan control actions (PETS) or generate synthetic rollouts for policy training (MBPO). We implement and couple these methods with the open-source simulator JutulDarcy, enabling flexible experimentation on waterflooding scenarios with multiple injectors and producers.

Our numerical experiments highlight distinct advantages and trade-offs of each MBRL approach. PETS achieves high data efficiency by iteratively refining action sequences through an uncertainty-aware planning routine but can occasionally settle in local optima under complex geology. In contrast, MBPO demonstrates robust performance in navigating high-dimensional control spaces, although it is more sensitive to hyperparameters and requires careful tuning to avoid training instabilities. Through ablation studies, we examine how key factors—such as planning horizon, surrogate model supervision length, and policy update frequency—affect convergence and policy quality in reservoir management tasks.

Overall, our results illustrate that MBRL provides a powerful framework for constructing computationally tractable proxy models and efficient control policies for porous media flow problems. These findings open new directions for RL applications in reservoir engineering, promising improved scalability and adaptability compared to classical optimization workflows.

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MS21 / 521

Permeation of semidilute polymer solutions through porous micromodels

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In civil engineering, it is common practise to support the walls of an open excavation, such as a borehole or trench, by filling it with fluid. The traditional and most widely used support fluids are slurries of bentonite clay in water. Semidilute aqueous solutions of high-molecular-weight polymer ("polymer fluids") are known have a variety of advantages over traditional bentonite slurries in terms of both cost and environmental impact, but they remain under-used because they are poorly understood. Here, we study the permeation of polymer fluids through porous micromodels to develop qualitative and quantitative insight into their flow through the pore space and their interactions with the solid skeleton. Our micromodels consist of custom microfluidic and millifluidic devices in a range of different geometries, complexities, and scales. We use a custom microscopy setup and a variety of imaging methods, including machine learning-assisted particle tracking velocimetry, to explore network-scale flow in 2D and pore-scale flow in 3D. Our working fluid is a semidilute aqueous solution of partially hydrolyzed polyacrylamide (HPAM). Dilute HPAM solutions have been widely studied in porous micromodels due to their well characterized shear-thinning rheology and relevance to many practical applications. At higher, semidilute concentrations, we find that entanglement and elasticity lead to hysteresis, transient effects, and a macroscopic pressure-drop-versus-flow-rate response that cannot be captured by simple shear rheology.

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522

Study on the occurrence characteristics of remaining oil after steam huff and puff in thin loose sandstone heavy oil reservoir

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Steam huff and puff plays a key role in the development of heavy oil reservoirs, especially super heavy oil reservoirs. At present, there are few studies on the variation of different components and the occurrence characteristics of remaining oil after steam huff and puff under the influence of different factors by combining micro and macro correlation.

Firstly, the one-dimensional visualization experiment combined with laser confocal microscope was used to analyze the residual oil occurrence state of the sample at different steam temperature and different steam cycles. Furthermore, some rock samples were selected to carry out nuclear magnetic resonance T2 spectrum test and core thin section observation experiment, and the occurrence state of remaining oil after steam stimulation was studied from the microscopic scale. Finally, based on the designed high-temperature and high-pressure two-dimensional proportional physical model, steam stimulation experiments were carried out to study the distribution of remaining oil after steam stimulation from a macro scale.

The results showed that after the first two rounds of steam stimulation, the light components in heavy oil were significantly reduced and the proportion of heavy components was increased. After

three rounds of huff and puff, obvious steam channeling channels could be seen, and the content of light components in the remaining oil was greatly reduced. After 5-7 rounds, there was almost no light component in heavy oil, and the remaining oil content changed little. With the increase of steam temperature, the remaining oil after 5 huff and puff cycles was obviously less, and the utilization degree of light components in crude oil was obviously improved. After 5 huff and puff cycles, the remaining oil was concentrated in the pores of 0.05 μm ~10 μm . The core slices could be seen under the microscope to form residual oil bands and steam channeling channels. In the early stage of steam huff and puff, the steam swept area of vertical wells advanced to the stable pressure wells with the huff and puff wells as the center, and the steam swept area of horizontal wells expanded evenly to the stable pressure wells with the huff and puff wells as the center, and the remaining oil was mainly distributed in the edge area of the model. After 7 rounds of huff and puff, it could be seen that obvious steam channeling channels were formed, and the remaining oil was distributed in the non-main streamline area; after 10 cycles of stimulation, the remaining oil was further reduced, but the decline was small.

The research results can better reveal the remaining oil occurrence characteristics and component change rules of steam stimulation in heavy oil reservoirs, and provide theoretical support for the selection and optimization of remaining oil development methods in the later stage.

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Water & Porous Media Focused Abstracts:

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References:

MS06-A / 523

Experimental evaluation of capillary retention of CO₂ in saline aquifers

Author: Rayana Peres^{None}

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Over the past 250 years, atmospheric CO₂ levels have increased markedly, rising from 270 to 370 parts per million (ppm), with half of this growth occurring within the last five decades. This trend is predominantly attributed to the intensified use of fossil fuels for energy production [1, 2]. Projections by the Organization for Economic Co-operation and Development (OECD) suggest that, without implementing effective mitigation measures, CO₂ emissions could rise by 70% by 2050. Such an increase is likely to drive global temperature rises of 3°C to 6°C by the end of this century [3]. This underscores the urgent need for strategies to control CO₂ emissions and limit the adverse environmental impacts of global warming.

Two primary approaches have been identified to address this challenge: transitioning from fossil fuels to renewable energy sources and adopting carbon capture and storage (CCS) technologies.

Among these, CCS stands out as one of the most effective tools for reducing CO₂ emissions in the short-to-medium term [4]. Estimates suggest that CCS could contribute nearly 20% to global emission reductions by 2050, while its exclusion might lead to a 70% increase in the global costs of meeting emission reduction targets [5].

Geological carbon storage (GCS) in saline aquifers has emerged as a promising long-term strategy for CO₂ sequestration. In this context, this study explores the feasibility of CO₂ injection and storage by capillary trapping in carbonate rocks through a core flooding experiment under high-pressure (8,000 PSIG) and high-temperature (91°C) conditions, simulating saline aquifer environments.

The experimental procedure involved saturating a low-permeability carbonate plug (Indiana Limestone) with NaCl brine at a concentration of 186 g/L. Subsequently, CO₂ gas was injected to displace the brine, maximizing gas storage. Finally, water was reinjected to displace the trapped gas and quantify the fraction of immobile gas.

The results confirmed the feasibility of saline aquifers as secure, long-term CO₂ storage sites. At 8,000 PSIG and 91°C, approximately 18% of the pore volume was occupied by immobilized CO₂ following water injection (Figure 1). This residual trapping demonstrates the rock's capacity to retain CO₂ securely, enhancing the stability of geological storage systems. The trapped CO₂ saturation was evaluated at different temperature values. These findings underscore the vital role of saline aquifers in advancing CCS initiatives and meeting global carbon reduction objectives.

Country:

Brazil

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Poster / 524

The synergistic role of pore geometry and wettability in governing immiscible displacement and entry capillary pressure

Author: Tongke Zhou¹

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Immiscible multi-phase flow within porous structures plays a crucial role in a variety of natural and industrial processes and is governed by several forces such as viscous, capillary, and buoyancy forces and pore geometry. Understanding the interplay of these factors is critical in controlling the behaviour of fluid-fluid interfaces in multi-phase flow in porous media. This interplay determines the resistance to fluid entry into pores and directly impacts the displacement efficiency. Entry capillary pressure is the capillary pressure that the nonwetting phase must overcome to enter a pore occupied entirely with the wetting phase. The effect of pore geometry and wettability on immiscible two-phase flow has been emphasised in recent research studies. However, the conventional entry capillary pressure equations neglect the three-dimensional (3D) details of pore structures and wettability, which results in deviations between analytical and practical results.

In this study, we adopted volume-of-fluid (VOF) method to explore the synergistic role of pore geometry and wettability in governing interfacial morphology, entry capillary pressure, and residual trapping. Numerical simulations were performed in four idealised constricted capillaries and two real pores extracted from rock sample. The numerical predictions were compared with analytical solutions and findings from other studies. The results show that entry capillary pressure temporarily decreases and even turns negative under intermediate wettability conditions during the drainage process when the interface initially enters the converging segment. Through the analysis of the evolution of interface morphology and the detailed distribution of curvatures on the interface, the role of net force rearrangement and pore geometry on evolution of curvature and displacement characteristics was investigated. Moreover, it was shown that intermediate wettability improves displacement efficiency due to curvature reversal (suction effect), which is also verified in core-scale experiments. This work highlights the importance of considering the corner flow in controlling immiscible two-phase flow dynamics in pore network modelling research.

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MS06-A / 526

Dynamics of brine drying and salt precipitation and growth in porous media during CO₂ injection

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Co-authors: Mehrdad Vasheghani Farahani ²; Javad Shokri ²; Vahid Niasar ²

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Subsurface CO₂ storage in deep saline aquifers, owing to their capacity, containment efficiency, and availability, is a promising strategy to enable the global net-zero target. Maintaining CO₂ injection into these storage sites is crucial for the success of carbon capture and storage (CCS) projects. However, dry CO₂ injection leads to brine evaporation in porous rock, resulting in salt precipitation once the concentration exceeds solubility limits, which may lead to dramatic injectivity loss.

Understanding the complex synergic effect of rock properties, injection parameters, and system thermodynamics on pore-scale brine drying and salt precipitation remains a challenge.

In this work, we conducted a series of microfluidic experiments to provide fundamental understanding of evaporation and salt precipitation in two-dimensional (2D) porous media. The experiments were conducted using custom-designed microfluidic chips with varying pore space heterogeneity, under atmospheric pressure and different temperatures and injection rates to shed light on key mechanisms controlling brine drying and salt precipitation in porous media. The results signify that (i) the residual brine distribution, determined by gas injection rate and pore structures, significantly controls the evaporation rate and salt distribution, (ii) depending on the injection rate and system temperature, two distinct types of salt crystal structures (monocrystalline structures nucleating within the aqueous phase and polycrystalline structures forming in the evaporated regions) may appear in porous media. The role of capillary backflow, driven by capillary pressure gradients during evaporation, was also elucidated in the context of salt crystallisation processes. This work provides a comprehensive understanding of the fundamental mechanisms of brine drying and salt precipitation, offering insights for optimising CO₂ injection strategies in saline aquifers.

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528

Investigating microscale processes in permafrost using microfluidic technology

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Permafrost contains 33% of the global carbon pool, making it an essential part of global carbon cycle, yet its microbial dynamics remain largely unexplored. Microorganisms in these environments face challenges, including freezing temperatures, low water availability, slow nutrient cycling, yet they play a critical role in regulating soil functions, such as the emission of greenhouse gases and the degradation of organic matter. Despite its importance, the microbial activity and metabolic processes in permafrost are not well understood.

The objective of this work is to assess biogeochemical processes at the microscopic scale resulting in CO₂ emissions from permafrost. To address the challenges of investigating these processes, we have developed a microfluidic platform, the “Permafrost-on-a-Chip,” designed to replicate the dynamics of the permafrost active layer. This device enables the investigation of microscale biogeochemical processes. The device integrates soil, microbes, and minerals, while mimicking freeze-thaw cycles. The microfluidic chip features a porous medium made of glass beads, which closely replicates permafrost seen as a porous medium. The design incorporates nutrient source chambers and porous media chamber providing a high-fidelity representation of soil structure. This layout allows for real-time visualization of microbial behaviors, including movement, accumulation near nutrient sources,

and interactions with soil particles, while simultaneously monitoring essential parameters such as temperature, moisture, and CO₂ concentration. Furthermore, the chip allows multiple tests to be conducted simultaneously, providing comparative data under various conditions.

This platform aids in exploring processes linked to greenhouse gas emissions and organic matter breakdown. By providing a detailed understanding of soil-microbe interactions in permafrost, the Permafrost-on-a-Chip technology marks a significant step forward in our understanding of microbial life in permafrost and will contribute valuable insights into climate change challenges.

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MS22 / 529

Deep Learning-Based Surrogate Model for Predicting Air Permeability of Technical Textiles

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The permeability of technical textiles is of crucial importance for industrial applications. It plays a key role in the development of high-performance fabrics as well as in the production of composite materials. In this context, porosity and structural properties have a much stronger influence on permeability than fibre composition, so the geometric design of the fabric is a more decisive factor than the choice of material. Air permeability is critical to fabric comfort, drying efficiency and production processes (such as drying itself), where the structure of the fabric can significantly affect performance. However, quantifying air permeability, especially for tightly woven fabrics, remains a challenge. Therefore, predicting permeability during the design phase can optimise production processes and minimise the need for extensive experimental testing. Liquid Composite Moulding (LCM) is a process for the production of fibre-reinforced composites in which dry fibre reinforcements are impregnated with low-viscosity resin. This process is subject to Darcy's law and is driven by the viscosity of the resin and the permeability of the material [\[1\]](#).

The aim of this project is to develop a surrogate model for permeability prediction based on deep learning techniques: in particular Fully Connected Neural Networks (FCNNs) and Convolutional Neural Networks (CNNs). These models are selected based on the desired output dimensionality: integral values or full-field spatial data. The model aims to predict the permeability from structural input parameters such as the weave type (plain weave, basket weave, filled rib and twill), cover factor (the ratio of the area covered by the fabric to the open area) and the aspect ratio (the shape ratio of the space between the yarns).

To achieve this goal, a training dataset was generated from CFD simulations performed for different geometries. These geometries differ in terms of weave pattern and yarn density and were generated using custom Python code implemented in the TexGen software API [\[2\]](#). A semi-automatic process was developed to investigate a wide range of geometric parameters, including mesh generation and adjustment of simulation settings. Permeability was calculated using Darcy's law under laminar flow conditions [\[3\]](#). This approach made it possible to evaluate the permeability through the air velocity flowing through the fabric.

Finally, the CFD models were refined and validated against experimental results from the existing

literature [4]. By combining CFD simulations with deep learning techniques, this study provides a powerful set of tools for the prediction of air permeability that facilitates the design and optimisation of technical textiles in various industrial applications.

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Poster / 530

Assessing water damage to gas permeability using bundle-of-tubes with triangular cross-section

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Water damage to gas permeability significantly impacts hydrocarbon recovery in gas reservoirs by altering the flow dynamics of gas and water phases within porous media. Addressing this challenge requires a deep understanding of fluid flow and distribution in porous structures to optimize hydrocarbon recovery strategies. Traditional bundle-of-tubes models often assume simplified circular pore geometries, which can lead to inaccuracies in predicting multiphase fluid flow and distribution. To overcome these limitations and enhance the accuracy of assessing water damage to gas permeability, a bundle-of-tubes model with triangular pore cross-sections was developed. By assuming that the cross-sections of all pores are equilateral triangles, a capillary pressure-non wetting phase saturation relationship was derived first for a single pore and then for a tube bundle. The types, quantities, and tortuosity of pores in the bundle were then adjusted to fit experimental mercury injection capillary pressure (MICP) curves and the actual porosity and permeability of the gas reservoir. The gas and water phases within the pores generated were distributed according to the wettability angles and surface tensions obtained from molecular simulations. Two distribution methods were investigated: one hypothesizes a uniform distribution of the wetting phase in all three corners of the pore under varying saturation and wettability conditions, and the other employs the lattice Boltzmann-Shan-Chen method to compute distributions of phases within the pore. Computational fluid dynamics (CFD) simulations were then conducted to evaluate gas permeability variations influenced by water saturation under both hypothetical and computed distribution scenarios. This study reveals that the wetting phase can distribute unevenly in the three corners of pores, rather than evenly as previously

assumed. This difference can generate rather significant effects on the quantification of the effect of water saturation on gas permeability.

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532

Leveraging Machine Learning to Optimize Well Placement for Geological CO₂ Storage and Utilization

Author: Jinjie Mao¹

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Multi-well placement optimization is a challenging task in the field development process of Geological CO₂ Storage and Utilization (GCSU), as the objective function is multi-dimensional, discontinuous, and multi-modal. Despite advancements in gradient-based and gradient-free optimization methods over the past decade, the complexity of geological systems continues to hinder effective well placement optimization. Furthermore, the application of high-fidelity physics-based models for well placement optimization exacerbates the challenge due to the computationally expensive nature of running thousands of numerical simulations. To address these issues, we employ data-driven models (DDM) using various machine learning (ML) approaches to predict reservoir responses based on injector and producer well locations. This enables strategic multi-well placement to optimize hydrocarbon recovery and CO₂ storage in partially depleted oil reservoirs while significantly reducing computational demands.

The Egg model serves as a benchmark case to validate the computational performance of DDM-based well placement optimization. Our formulation is focused on the CO₂ water-altering-gas (WAG) operation, with well locations as input parameters and net cash flow (NCF) as the output after a specified operational period. Training datasets are generated using Quality Map (QM)-constrained random sampling (RS), with input features including well coordinates, permeabilities, porosities, initial saturations, pressures, time of flight (TOF), and well-to-well distances, while outputs capture cumulative oil, water, and CO₂ production. We evaluate the strengths and limitations of various ML methods, including Multiple Perceptron (MLP), Extreme Gradient Boosting (XGBoost), and Deep Neural Networks (DNN), across different sizes of training and testing datasets. All these models achieved R^2 values exceeding 0.97, delivering fast and accurate predictions. Among them, MLP-based proxies stood out for their superior accuracy and computational efficiency, especially when applied to larger datasets.

Integrating the MLP model built upon 1,100 datapoints into a genetic algorithm (GA) allows effective optimization of the injector and producer locations in the studied heterogeneous, three-dimensional reservoir, with net cash flow (NCF) as the objective function. The MLP-GA outperforms traditional simulator-based GA optimization by improving computational efficiency threefold while achieving similar optimal well locations and NCF values, thereby supporting sustainable subsurface resource utilization.

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Norway

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Evaluating the Pressure Dependence of the Longitudinal Modulus of an Adsorbate in Nanopores Using Ultrasound: A Novel Procedure Taking the Effect of Emptying Pore Ends into Account

Authors: Klaus Schappert¹; Rolf Pelster¹¹ *Universität des Saarlandes, Department of Physics***Corresponding Authors:** k.schappert@mx.uni-saarland.de, rolf.pelster@mx.uni-saarland.de

Nanoconfinement can influence the elasticity of adsorbed substances [1,2]. Generally, the determination of the elastic moduli of nanoconfined substances from measured effective quantities is a challenging task [1,2]. Here we explore the possibilities to determine an adsorbate's elastic modulus and its pressure dependence using ultrasound. As a model system, we study the isothermal adsorption and desorption of liquid argon in nanoporous glass with an average pore diameter of $d_P = 25.6$ nm. The longitudinal modulus of an adsorbate, β_{ads} , is usually determined by means of an effective medium equation using the average modulus of the filled porous system, $\beta_{av} = c_l^2 \rho$, with c_l being the measured velocity of longitudinal ultrasonic pulses propagating through the sample and ρ the average density. However, in the so-called plateau region of a sorption isotherm, curved liquid-vapor menisci and empty pore ends are present at the outer surface of the sample, i.e., the filling of the pores and the density vary within the sample. With the analysis of our ultrasonic measurements, we show that the determination of the pressure dependence of an adsorbate's modulus requires the careful consideration of the accurate geometrical arrangement of the adsorbate in the volume, where the ultrasonic pulses propagate. Thereby, we have developed a method for the correct determination of the pressure dependence of an adsorbate's modulus that can be applied to other porous systems. Thus, our findings will have an immediate impact on the interpretation and analysis of ultrasonic studies on elastic properties of nanoconfined materials [3].

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Pelster, R. Elasticity and Phase Behavior of Fluids in Nanoporous Media. In *Soft Matter and Biomaterials on the Nanoscale: The WSPC Reference on Functional Nanomaterials, Part I, Volume 1: Soft Matter under Geometrical Confinement: From Fundamentals at Planar Surfaces and Interfaces to Functionalities of Nanoporous Materials*, Huber, P.; Gang, O.; Spaepen, F., Eds.; World Scientific: Singapore, 2020; Vol. 20, pp. 259–304. [3] Schappert, K.; Pelster, R., Evaluating the Pressure Dependence of the Longitudinal Modulus of an Adsorbate in Nanopores Using Ultrasound: A Novel Procedure Taking the Effect of Emptying Pore Ends into Account, *J. Phys. Chem. C* 128, 21081–21089 (2024).

Poster / 535

Microscale Processes, Macroscale Solutions: Biofilms in Sustainable Water Filtration

Author: Mandana Samari-Kermani¹

Co-authors: Enno de Vries²; Matthijs de Winter¹; Jack Schijven¹; Amir Raoof¹

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The increasing global demand for safe drinking water emphasizes the importance of energy-efficient and sustainable treatment technologies such as slow sand filtration (SSF). Central to SSF's efficacy is the bioactive layer, or Schmutzdecke (SD), which facilitates particle removal through biological and physical processes. This study bridges microscale insights into biofilm dynamics with macroscale filtration performance, advancing our understanding of SSF optimization.

The research investigates the impact of operational parameters, such as sand grain size and material, on SD development and SSF performance. Fine-grain sand filters were found to promote faster SD formation, enhancing microbial activity and particle retention. A key finding was the role of the protein-to-carbohydrate ratio within the SD as a critical indicator of *Escherichia coli* removal efficiency. To uncover the mechanisms underlying particle removal, microfluidic experiments with realistic pore structures were conducted using 1.5 µm fluorescent particles and biofilms of varying maturity. Advanced fluorescent microscopy and confocal laser scanning microscopy enabled direct observation of biofilm growth, particle transport, and removal mechanisms at pore-scale resolution.

The results demonstrated that biofilm growth significantly alters porous media properties, including pore size distribution, hydraulic conductivity, and effective porosity. As biofilm matured, preferential flow paths emerged in the porous media, increasing particle velocities from 4.58 mm/s in clean conditions to 7.4 mm/s in bio-clogged conditions. This hydrodynamic shift created isolated zones and enhanced straining mechanisms, resulting in over 50-fold reduction in hydraulic conductivity and a decrease in effective porosity from 36% to 9%. Consequently, the fraction of permanently attached particles increased significantly, improving log₁₀ removal efficiency of the sand [1](#).

At the macroscale, these findings align with observed improvements in SSF performance under mature SD conditions. The study highlights that biofilm-induced surface roughness and pore structure modifications enhance particle retention by developing low-velocity zones favourable to attachment. Furthermore, increased tortuosity due to biofilm growth redirected flow through preferential paths, amplifying particle capture efficiency.

This research provides a comprehensive framework for understanding the interplay between biofilm development and filtration performance across scales. By elucidating the mechanisms driving particle removal in SSF systems, it offers actionable insights for optimizing operational parameters to ensure safe drinking water production while maintaining filter longevity.

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References:

1 Samari-Kermani, M., de Vries, E. T., Schijven, J. F., & Raoof, A. (2024). A closer look at the role of biofilms in water filtration: Bridging microscopic insights with system performance. *Journal of Water Process Engineering*, 67, 106104. <https://doi.org/10.1016/j.jwpe.2024.106104>

Poster / 536

High-pressure and High-temperature Fluid Flow system in the MOGNO Beamline for Time-Resolved Tomography

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The fourth-generation synchrotron facility provides X-rays from low to high energy with a high flux of photons that, coupled with advanced detector technology, allow routine acquisition of high-resolution tomograms in a few seconds. In addition to high-throughput experiments, in this case, computed tomography can also be resolved in time, which is the 4D CT scan. Among the wide range of interesting physical phenomena to be solved in time by three-dimensional images, the fluid flow in porous materials is one that is present in several areas, such as oil industry, agriculture, and environmental science. In particular, the flow of fluids in very deep reservoirs is an important scientific case, where the porous material is under very high pressure (HP) and, normally, also at high temperatures (HT). With that in mind, the MOGNO group, in partnership with the energy company Equinor and Petrobras, is installing an HPHT Fluid Flow system at the beamline. This work aims to show the scientific community the system to be installed, promote discussions about the device and future experiments, such as time-resolved fluid flow in porous media, and take this perspective to other areas of knowledge. MOGNO is an imaging beamline designed to deliver micro and nano computed tomography, focused on multi-scale analysis (zoom tomography) **1**, and 4D imaging (time-resolved 3D) **2** through in-situ experiments. The analysis of rock cores is vital in various areas, including energy, CO₂ sequestration, and understanding Earth's evolution. To meet these specifications and study such materials, the MOGNO beamline was designed with three different energy levels and a high photon flux.

Experimental setup: Fluid flow is among the most challenging processes to observe in 3D and in situ, especially concerning spatial and temporal resolution. Addressing this challenge, the MOGNO group, in partnership with Equinor and Petrobras, is currently installing a high-pressure (HP) and high-temperature (HT) Fluid Flow system with the following key features:

- Confining pressure of up to 15k psi for specific core holders.
- Operating temperature capacity up to 90°C.
- Achieving temporal resolution in the order of seconds.
- Samples with a diameter of 12 mm and 1 inch.
- Simultaneous injection of two fluids for experimental flexibility.
- Prepared for both: high salinity seawater and crude-oil.
- Offers options for top/bottom and bottom/top injection configurations.

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Poster / 537

Understanding the role of cryosuction on flow and transport in partially frozen porous media

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Freeze-thaw cycles are ubiquitous in cold climates and can affect groundwater recharge and solute transport through the porous subsurface. These cycles create freezing and melting fronts that propagate centimeters to meters into the vadose zone. Within the vadose zone, these fronts cause spatial and temporal variations in pressure and temperature that impact flow and transport. These coupled hydrologic, mechanical, and thermodynamic changes drive a range of complex processes including cryosuction, solute quenching, and pore space expansion. In partially saturated porous soils experiencing freezing temperatures, ice content increases, which in turn causes the capillary pressure in the partially frozen media to increase. This dynamic capillary pressure change causes fluid to migrate upwards, a phenomenon known as cryosuction. While freeze-thaw cycles and their associated processes are frequent in high latitude regions, a key knowledge gap exists in how cryosuction processes affect groundwater recharge and the mobility and distribution of contaminants within the vadose zone.

To quantify the influence of freeze-thaw cycles, we created a quasi-3-dimensional tank (Hele-Shaw cell) filled with glass beads to act as the porous media. The tank was first partially saturated with unfrozen water and subsequently frozen using a circulating system to generate a top-down freezing front. To track the movement of fluid flow, we added a dye tracer to the unfrozen bottom layer of the tank. Time lapse photography recorded the movement of the dye tracer throughout experimental trials and was used to optically visualize the cryosuction-driven transport within the bead pack

during freezing front progression. Image processing was used to quantify liquid water content and tracer movement to interpret the role of cryosuction-driven transport. The results of this study provide valuable insights into cryosuction processes in unsaturated porous media, as well as water quality and recharge of near-surface aquifers in areas that experience seasonal freezing.

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MS26 / 538

How to Best Model Multiscale Capillary Heterogeneity for Geologic CO₂ Storage

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Objectives and Scope

The impact of capillary heterogeneity on CO₂ multiphase flow behavior has been increasingly recognized in the past decade. Ranging from millimeter to kilometer scale, capillary barriers are prevalent in the subsurface. They can be formed wherever geologic heterogeneity exists, from slight variation in the sand grain sizes, to an extensive sequence of interbedded sand and shale. Because capillary heterogeneity is multiscale, its influence on CO₂ flow and trapping also carries across scales. Therefore, it is important for practitioners to better understand and model capillary heterogeneity for CO₂ storage.

Methods, Procedures, Process

We conducted a review on pertinent literatures and elaborated key observations from the core to field scales. For example, experimental studies have shown that millimeter-decimeter scale capillary heterogeneity can cause above-residual capillary trapping known as capillary heterogeneity trapping. Capillary heterogeneity at this scale can also lead to complex upscaled constitutive relationships under capillary-dominated flow regimes, such as flow-rate dependent and anisotropic relative permeability as well as non-conventional initial-residual saturation relationships. Furthermore, under gravity-dominated flow regimes, centimeter-meter scale capillary heterogeneity can entrap a significant amount of CO₂ not just after imbibition, but also during drainage. The presence of capillary heterogeneity can even completely arrest the vertical movement of CO₂ plume, hence not only greatly reducing leakage risks, but also demonstrating the feasibility of an alternative confining system to traditional continuous seal/cap rocks.

Results, Observations, Conclusions

To accurately model the influence of capillary heterogeneity on CO₂ plume migration and retention at the field scale, a geologically realistic earth model is needed to ensure the proper representation of capillary heterogeneity across various scales, especially the larger-scale heterogeneity. At smaller

scales, capillary effects should also be emphasized so that constitutive multiphase flow relationships affected by small-scale capillary heterogeneity can be properly upscaled.

Significance/Novelty

In this work, we present our best theoretical recommendation for a step-by-step workflow on how to preserve capillary heterogeneity across scales in order to increase accuracy when modeling CO₂ plume migration and trapping in storage aquifers based on the literature reviewed.

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MS09 / 539

Mechanisms of interface jumps, pinning and hysteresis during imbibition and drainage along an isolated pore

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Co-authors: Ivan Lunati ²; Jordi Ortín ³; Juan J. Hidalgo ⁴; Marco Dentz ⁴

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We study experimentally and numerically the mechanisms of interfacial jumps, pinning and capillary hysteresis along an elementary pore. To this end, we analyze quasi-static fluid imbibition and drainage cycles in a capillary tube with conical constrictions (ink-bottle). Depending on the slope of the conical section, we observe a range of interfacial behaviors, including capillary jumps, and interface pinning during both imbibition and drainage, which give rise to capillary hysteresis, that is, history dependence of the interface position.

A theoretical model based on pressure balance at the interface captures the full spectrum of behaviors in terms of the pore geometry, contact angle and surface tension.

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Solute transport in a shear-thinning fluid flow through porous media**Author:** Amna Al-Qenae^{None}**Co-authors:** Javad Shokri¹; Muhammad Sahimi²; Takshak Shende³; Vahid Niasar¹¹ *University of Manchester*² *University of Southern California*³ *University College London***Corresponding Authors:** mohammadjavad.shokriafr@postgrad.manchester.ac.uk, moe@usc.edu, vahid.niasar@manchester.ac.uk, takshak.shende@gmail.com, amna.al-qenae@postgrad.manchester.ac.uk

The flow of non-Newtonian fluids in porous materials can be found in many industrial applications such as chemical engineering, subsurface engineering (de-contamination, energy production), and the food industry.

The relation between the shear stress and viscosity in non-Newtonian fluids is not linear and it is time-dependent, making it difficult to understand their behaviour. Non-Newtonian shear-thinning fluids tend to decrease in viscosity as the shear rate increases, while non-Newtonian shear-thickening fluids tend to increase in viscosity as the shear rate increases. The process of transporting non-Newtonian fluids through porous materials is complicated and influenced by different factors. These factors include the properties of the fluid, the porous material, and the flow conditions. The fluid flow rate is impacted by the fluid's velocity, pressure gradient, and the porous medium's tortuosity. Extensive research has shown that the properties of the fluid, the porous material, and the flow conditions all play a significant role in transporting shear-thinning fluids through porous media.

The present study uses a laboratory approach to examine the flow of a non-Newtonian shear-thinning fluid in a porous media. The fluid bulk rheology was obtained from the rheometer measurement first to confirm the viscosity-shear relation for the selected non-Newtonian fluid (xanthan gum), and the results were fitted using the Meter model equation. Then, a microfluidic experiment was done using xanthan gum solution mixed with a water-based ink colour to act as a tracer in the porous medium to track the fluid movement and breakthrough path. The experiment was done using different injection flow rates. The images were recorded during the experiment and processed after each experiment to calculate the average effluent concentration versus time and estimate the dispersion coefficient using Ogata and Banks' equation. The results showed a non-monotonic behaviour for the non-Newtonian fluid flow in porous media.

Country:

United Kingdom

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

Mesoscale modeling of electrochemical reactive transport in Unitized Reversible Fuel Cells

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Global climate change is a pressing issue that has prompted humankind to reduce the overutilization of fossil fuels to fulfill their energy demands. Accordingly, renewable energy sources, such as wind, solar, and geothermal have gained significant attention in recent years, catering to an ever-increasing proportion of the overall energy supply chain. However, the intermittent nature of these renewable sources precludes their continuous application, thereby leading to the introduction of secondary batteries or reversible fuel cells (RFCs) in the energy mix for long-duration storage [1]. Polymer Electrolyte Membrane Unitized Reversible Fuel Cells (PEM-URFCs) is an environmentally benign electrochemical device that offers round-trip energy conversion by integrating a fuel cell (FC) mode with an electrolysis cell (EC) mode. Owing to its distinct advantages, such as high specific energy density, compact design, and zero tailpipe emissions, PEM-URFCs are used in a gamut of applications such as spacecraft, solar rechargeable aircraft, and residential power sources [2]. As the pursuit to develop next-generation PEM-URFCs continues, optimizing the porous catalyst layer (CL) design –primarily the oxygen electrode, which hosts the sluggish oxygen reduction reaction (FC mode), and oxygen evolution reaction (EC mode) is essential. Particularly important is controlling the microfluidics of fluid flow at the interfaces (water drainage for FC vs supplement for EC mode), which depends on a detailed mechanistic understanding of the multiphase reactive transport interactions occurring within the CLs. In this work, we present a mesoscale modeling framework to probe the electrochemical landscape of the PEM-URFC. The input to this workflow is stochastically generated realistic CL structures with various microstructural attributes such as pore size, ionomer content, and electrode thickness. Reactive transport simulations employing pore-network modeling [3] are subsequently performed on these structures to analyze the underlying electrochemical signatures. We further reveal the influence of CL structural parameters on the resulting ohmic overpotentials and mass transport limitations within a wide range of operating conditions. A mesoscale optimization study demonstrated in this work aims at unraveling the intricate structure-transport-process-performance relationships in the catalyst layers of PEM-URFCs.

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United States

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Water & Porous Media Focused Abstracts:

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Microfluidic analysis of N₂O cycling in karst aquatic systems: Linking hydrological, geochemical and microbiological processes

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Karst landscapes, comprising ~20% of the Earth's ice-free land surface, are geological terrains characterized by topographical features resulting from the dissolution of soluble rocks, primarily carbonates. These dissolution features, such as sinkholes and conduits, facilitate the interaction between surface water and groundwater, making the hydrological and biogeochemical characteristics of karst landscapes a crucial component of the global nitrogen (N) cycle. Specifically, karst landscapes and aquifers have recently been identified as hotspots for the production of nitrous oxide (N₂O), the third most important greenhouse gas with a 100-year global warming potential ~300 times that of carbon dioxide. However, the mechanisms by which N₂O is produced and consumed across karst aquatic landscapes remain poorly understood due to a variety of heterogeneous, yet often coupled, hydrologic, chemical, and microbiological processes that influence N₂O cycling. Thus, a holistic approach that considers the interplay between these processes is necessary to quantitatively predict N₂O production and consumption rates within, as well as emissions from, karst aquatic environments. Such advances are essential for developing predictive models of future global warming, for which N₂O production is likely to have a major impact because (1) reactive nitrogen species, such as nitrate (NO₃⁻) and ammonium (NH₄⁺), which microbes convert to N₂O, have more than doubled in aquatic environments over the past few decades due to anthropogenic activities (e.g., fertilizer use, fossil fuel burning), and (2) karst landscapes are globally widespread. We present a microfluidic study where we (1) develop microfluidic chips that replicate karst aquifers to simulate various hydrologic conditions, (2) use the microfluidic chips to experimentally produce and measure N₂O production and consumption by inoculating and culturing denitrifying bacteria under various hydrologic conditions, (3) measure functional gene activity to identify dominant microbial processes responsible for N₂O cycling, and (4) link lab experimental findings to field measurements including nitrogen species concentrations, microbial activity, and hydrological conditions to evaluate natural N₂O production and consumption mechanisms. The results show that (1) surface water-groundwater interactions create conditions favorable for N₂O production through incomplete denitrification and (2) the magnitude and duration of such interactions controls both N₂O production and consumption rates and therefore, atmospheric emissions from karst aquatic ecosystems.

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References:

MS26 / 543

Capillary trapping and flow dynamics in CO₂-Brine systems: A Microfluidic experimental study near the critical point

Authors: Brenda Maria De Castro Costa¹; Jorge Avendaño²; Yan Salema de Medeiros³

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Efficient carbon capture and sequestration (CCS) in deep saline aquifers relies on understanding the complex interactions between CO₂ and brine under varying conditions. Previous studies have provided critical insights into the mechanisms driving CO₂ storage. For instance, Wildenschild et al. [1] quantified the effects of interfacial tension, viscosity, and flow rate on capillary trapping, while Pentland et al [2] measured the residual non-wetting phase saturations of supercritical CO₂, emphasizing capillary trapping as an effective immobilization mechanism. Furthermore, Peichung et al [3]. demonstrated how high-pressure microfluidic experiments enhance mass transfer rates, offering key insights into multiphase flow dynamics.

Considering relevant factors on these studies, we investigate the injection of CO₂ into a porous media micromodel, alternating with brine flooding, as a promising strategy to better understand carbon sequestration. This study examines the impact of pressure conditions—above and below the critical point of CO₂—on multiphase flow dynamics and CO₂ storage efficiency in saline aquifers. Using the Sapphire Lab microfluidic platform, we conduct controlled experiments that allow precise regulation of flow rate, pressure, and temperature, while simultaneously visualizing fluid behavior in the micromodel.

This approach enables real-time monitoring of aqueous phase saturation throughout the injection process, capturing the interplay between CO₂ and brine phases under diverse thermodynamic conditions. Key phenomena such as saturation, displacement patterns and capillary trapping are analyzed to understand the influence of sub- and supercritical pressures on fluid distribution and storage mechanisms.

Preliminary results reveal distinct behaviors at pressures above and below the critical point, with significant implications for optimizing injection strategies. High-resolution microfluidic techniques enhance the accuracy of multiphase flow observations, providing valuable insights for designing more efficient and sustainable carbon storage operations.

Country:

Brasil

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Student Awards:

Water & Porous Media Focused Abstracts:

This abstract is related to Water

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MS20 / 544

Towards a Predictive Model for Vertebral Failure: Coupled Tumour Growth and Bone Remodeling Framework

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Bone metastases, particularly in the spine, present a significant clinical challenge as they weaken the structural integrity of vertebrae, increasing the risk of fractures and spinal cord injuries. Tumours disrupt the normal balance of bone remodelling through a complex interplay of molecular signalling, biochemical changes, and mechanical forces, resulting in lesions characterized by excessive bone resorption or formation. Therefore, to accurately predict bone failure, it is essential to first model tumour growth and its effect on bone formation and resorption.

This work aims to develop a mathematical model to predict vertebral failure by first constructing a coupled tumour growth and bone remodelling framework. The tumour environment is treated as a porous medium where the different cell populations are assumed to behave as viscous fluids. The deformable bone matrix constitutes the solid scaffold, while the pore space is saturated by the tumour cells, host cells and the interstitial fluid. The tumour cell phase is further split between two species: living tumour cells and necrotic ones. We also account for cells metabolism and oxygenation by adding an oxygen specie in the interstitial fluid phase.

However, to investigate the impact of the tumour on bone formation and resorption, additional species need to be incorporated into the multiphase system. Specifically, two cell populations—osteoblasts and osteoclasts—must be included within the host cells phase. Additionally, two signalling molecules, RANKL and OPG, which regulate the differentiation and activation of these cells, must be introduced as species within the interstitial fluid phase.

The coupling of the tumour growth and bone remodelling models enables the prediction of microstructural evolution over time. By linking this evolution to the bone's mechanical properties, it becomes possible to run damage mechanics models to predict crack initiation and propagation in the vertebrae, thereby facilitating the characterization of fracture risk.

Starting from the general conservation equations of mass and momentum derived using the Thermodynamically Constrained Averaging Theory (TCAT), we formulate the mathematical model for the coupled tumour-bone system, resulting in a system of Partial Differential Equations (PDEs). This system is numerically solved using the Finite Element Method (FEM) Firedrake software.

The model is applied to patient-specific geometries obtained from labelled CT scans, and the resulting fields of mechanical properties are used as inputs for a damage mechanics model to simulate fracture initiation and propagation under various loading scenarios. Finally, the parameterisation of the model to adapt it to patient-specific settings will be discussed, along with its potential application in supporting medical decision-making.

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References:

Poster / 545

High-Resolution Computed Tomography Dataset of Mount Simon Sandstone

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Geological carbon storage is an essential part of climate change mitigation. The Illinois Basin has become an early focal point of geological carbon storage (GCS) research and its implementation in the United States. The principal storage target in the basin is the Mount Simon Sandstone. Known for its exceptional thickness, depth, porosity, and sealing properties of overlying formations, this saline reservoir is crucial for long-term CO₂ sequestration efforts.

In support of these efforts, we present an extensive Computed Tomography (CT) dataset on a high porosity and permeability zone in the lower Mount Simon Sandstone available on the Energy Data eXchange® (EDX). This publicly accessible database comprises over 500 GB of high-resolution CT scans of six core samples, with resolutions ranging from 14.8 µm to 0.7 µm per pixel. The scans include both dry sandstone samples and those saturated with brine and supercritical CO₂, allowing for comparative analyses across different conditions and resolutions. Coarser scans provide an overview of the sandstone's bedding structure, whereas finer resolution scans reveal intricate details of pore infill and pore throat features. Metadata on location, depth, and saturation state enhance usability, enabling quick identification and cross-sample comparisons.

This dataset represents over a decade of non-destructive geological characterization work, consolidating results from various projects into a single, accessible resource. This data repository can inform permeability models and refine predictions for reservoir performance. Dissemination of this information to the wider scientific and GCS community will support further model development, testing, and stakeholder engagement. By providing a robust resource for research and collaboration, the database contributes to achieving net-zero greenhouse gas emissions by supporting continued progress in safe, reliable, and environmentally sustainable energy solutions.

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Gill, M., Pohl, M., Brown, S., Jarvis, K., Crandall, D. Mt. Simon Sandstone - High Resolution CT. Energy Data eXchange, 2024. <https://edx.netl.doe.gov/dataset/mt-simon-sandstone-high-resolution-ct>, DOI: 10.18141/2326948

MS09 / 546

Pore-scale level-set simulation of drainage-imbibition cycles of trapped gas during decline and incline of reservoir pressure

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New uses of subsurface reservoirs such as temporary storage of natural gas and hydrogen, involve seasonal gas injection and production schedules accompanied by seasonal inclines and declines in reservoir pressure, respectively. In the gas withdrawal stage, rising water will trap gas in the gas/water transition zone below the producing gas cap. The injection and production of gas leads to drainage and imbibition processes in the reservoir which traditionally have been studied by two-phase displacement of continuous flow of gas and water at the pore scale. Here, we will instead focus on the drainage and imbibition characteristics that occur due to the expansion and compression of the trapped gas when the reservoir pressure changes.

To this end, we use a level set model for capillary-controlled displacement with local volume conservation as a basis for the investigations [1]. The model enforces volume conservation of disconnected ganglia by modifying their pressure (that is, the normal level-set velocity) to prevent volume changes, and it also conserves volume during ganglion splitting and merging. Thus, simulations predict the pressures of trapped ganglia, which is a prerequisite for describing pressure-volume behaviour of ganglia under various processes, such as Ostwald ripening of trapped gas [2]. Here, we extend the model to handle local mass conservation of a compressible gas when the (uniform) reservoir pressure changes stepwise. The strategy is to first calculate the equilibrium gas pressures for trapped ganglia from which we calculate the number of moles of gas from an equation of state (EOS). Then, for each stepwise change in reservoir pressure, we combine the EOS with the volume conservation equation to find the gas pressure in each level set iteration that corresponds to the volume for the current reservoir pressure. In case of Peng-Robinson EOS the resulting pressure equation is a fourth order polynomial which we solve either numerically or analytically in each level set iteration. The reservoir pressure is changed once a static fluid configuration is achieved.

Using the developed model, we perform quasi-static simulation of pressure incline followed by pressure decline on trapped gas configurations after imbibition on a 3D segmented micro-CT image of sandstone. We monitor changes in average ganglion pressure as a function of trapped gas saturation and show the hysteresis behaviour. The simulations also show that pressure incline results in snap-off of large ganglia as they get compressed. Further, both coalescence and snap-off are observed during pressure decline when ganglia grow and extend into nearby pores.

Country:

Norway

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MS06-A / 547

Interpretation of an Interwell Partitioning Tracer Test in a Multi-layer Carbonate Reservoir

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Interwell Partitioning Tracer Test (IPTT) estimates remaining oil for economic evaluation of reservoir operations. It involves waterflooding and co-injection of two chemicals: one that is water-soluble (conservative) and another that also partitions into the oil phase. The downstream concentration of injected chemicals yields concentration history (CH). Cooke's interpretation of CH estimates remaining oil from tracer arrival times. Complex reservoirs need extra interpretation effort. This study reanalyzes IPTT data from a giant Saudi Arabian reservoir, as published by Sanni et al. (2016).

We introduce the following complexities of an oil reservoir: multi-layer structure, mass-transfer resistances, and stagnant zones. We combine them in a physically reasonable way to capture the first-order effects.

We use the well-known advection-dispersion equation (ADE) with extra terms for each of the complexities. Partitioning tracer transport is modeled with an ADE and mass-transfer resistance to the stagnant oil phase in each layer. The oil phase is continuous and allows for partitioning tracer communication between the layers. The conservative tracer follows classic ADE in both layers. The system of differential equations is solved numerically with COMSOL.

Remaining oil saturation presented in Sanni et al. (2016) was ~ 0.2 , while missing half of the partitioning tracer mass. The model shows a good fit of partitioning tracer at early times, and notably lower quality fit at late times. This result was obtained using a non-mass conservative analytic solution fitted to the data independently for conservative and partitioning tracers thus ignoring continuity of physical properties of the formation.

Conversely, our model preserves such continuity by fitting only one dual-layer mass-conservative model with partitioning tracer transport between the layers. Consequently, our model accounts for all recovered mass for both conservative and partitioning tracers. The oil saturation obtained by our model is 0.17 in the first layer and 0.2 in the second layer. The saturation in the two layers indicates microscopically trapped oil that reached residual saturation. While the oil saturation in two layers is similar to the original result, the existence of an extra oil rich layer explains the late time data much better than the original model. Figure 1 shows the breakthrough curves with the IPTT data, the original report model (blue dotted line), and our proposed model (blue dashed line), both for partitioning tracer.

For the first time, we interpret IPTT data for a multi-layer reservoir with stagnant zones, inter-layer oil communication, and slow partitioning tracer diffusion in oil phase. Our analysis reveals hydrocarbons in a second layer, missed in the original report. This study demonstrates proper physics-based test interpretation and provides guidance on essential data collection to improve IPTT analyses.

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Saudi Arabia

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Modiu Sanni et al. "Pushing the Envelope of Residual Oil Measurement: A Field Case Study of a New Class of Inter-Well Chemical Tracers". Society of Petroleum Engineers (2016). DOI: 10.2118/181324-MS.

MS06-A / 548

Fluid-fluid interface dynamics in an imperfect Hele-Shaw cell: A novel computational method for hysteresis and energy dissipation

Authors: Mykyta V. Chubynsky¹; Marco Dentz²; Jordi Ortín³; Ran Holtzman¹

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In a cylindrical capillary or a Hele-Shaw cell with perfectly flat walls, the equilibrium position of the interface between two fluids given the external conditions such as the pressure head is unique. If the external conditions change infinitely slowly (quasistatically), the interface follows this equilibrium, thus, its position is history-independent; there is no energy dissipation in this quasistatic limit. In contrast, in disordered porous and fractured media there are multiple equilibria, leading to history dependence (hysteresis) of the interface evolution even in the quasistatic limit, and Haines jumps of the interface between these equilibria lead to dissipation. An imperfect Hele-Shaw cell (with a gap width randomly varying in space) provides a simple model system in which these phenomena (both in the quasistatic limit and beyond) can be studied, promoting understanding of multiphase flow in a rough fracture as well as providing insights into more complex, 3D porous media. However, even in this simple model the evolution of the interface is nontrivial due to the nonlocality brought about by the resulting fluid flow, which, in principle, requires solving the Stokes equations for the flow in the whole domain even when only the interface evolution is of interest.

We present a novel spectral approach for computing the interface evolution in such a system, based on the Fourier expansion of the interface shape at each time step, confirming its accuracy via comparison to the much more computationally costly numerical solutions of the Stokes equations. We use our approach to study the (microscopic) dynamics of the interface relaxation towards equilibrium, as well as the (macroscopic) pressure-saturation trajectories following drainage/imbibition cycles. We find that even for a single perturbation ("defect") in an otherwise perfectly uniform cell, interface relaxation dynamics in a Haines jump is a complex, multistage process. Nonetheless, we present a remarkably simple model relying on the concepts of viscous and "dry friction" dissipation, that is able to predict the pressure-saturation cycles in random media. Our findings are a promising step towards an upscaled model of flows in rough fractures, where from the macroscale properties of the roughness one could obtain the averaged interface dynamics.

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Poster / 549

Brady's Geothermal Field Computed Tomography Core Characterization

Authors: Magdalena Gill¹; Sarah Brown²; Karl Jarvis³; Laura Dalton⁴; Dustin Crandall³

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Enhanced geothermal systems (EGS) are an integral part of the expanding renewable energy portfolio and hold the promise of deploying geothermal energy sources beyond traditional areas. Optimizing injection strategies and the placement of new wells in existing and prospective hydrothermal fields requires a thorough understanding of fluid and temperature distribution in fractured subsurface reservoirs. However, limited public data exist for natural or enhanced hydrothermal systems, hindering the ability to develop optimized strategies for reservoir development and stimulation to effectively expand geothermal energy production.

Brady's Geothermal Field in northwestern Nevada, which has been producing power since 1992, was the site of an early EGS demonstration aimed at testing potential production expansion into near-field unproductive wells (Akerley et al., 2020). While the project failed to make the target well productive, it involved extensive data collection and characterization during the pre-stimulation phase.

We present a publicly accessible database centered around multi-scale Computed Tomographic (CT) imaging of samples from the BCH-03 well, supplemented by a wide range of supporting geological analyses (Brown, et al., 2022). The data include detailed petrologic descriptions of core samples, core-scale medical CT scans, high-resolution micro-CT scans, thin section photomicrographs, elemental abundance data from X-ray diffraction, velocity wave measurements, and helium porosimetry of the matrix.

The multiple data streams enable ground-truthing and validation of digitally derived porosity values by cross-referencing with experimental porosimetry results and thin section estimates. Additionally, the multi-scale nature of the dataset allows for evaluation of both matrix and fracture porosity, permeability, and morphology. This facilitates data upscaling for model development and testing, as well as correlation with adjacent well data to enhance field-scale understanding of subsurface fracture networks, connectivity, and controls on fluid flow.

This comprehensive dataset, hosted on the government- and National Energy Technology Laboratory-maintained Energy Data eXchange (EDX), advances our understanding of influential factors on subsurface hydraulic connectivity. Such insights are critical for enabling successful expansion and development of hydrothermal energy resources in the future.

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MS15 / 550

Artificial Intelligence for Predicting and Accelerating Reactive Contaminant Transport in Porous Media

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Porous media, such as soils and aquifers, play a crucial role in various environmental and industrial processes, including groundwater management, pollution control, and resource extraction. Modeling the transport of reactive contaminants within these media involves complex interactions between physical properties (e.g., porosity and permeability) and chemical reactions. Traditional numerical simulation methods, though effective, are often computationally expensive and face difficulties in efficiently resolving the nonlinear, coupled interactions that characterize these processes.

This study addresses these challenges by applying Artificial Intelligence (AI) techniques to enhance the simulation of reactive contaminant transport in porous media. The underlying problem is modeled by a system of nonlinear partial differential equations describing diffusion-convection processes, coupled with algebraic equations representing chemical equilibria. A key computational bottleneck arises from the chemical reaction calculations, which require significantly more computational resources than the transport simulations.

To mitigate this, the study integrates machine learning and AI algorithms to predict and accelerate these simulations, achieving both high accuracy and reduced computational costs. Deep learning models, trained on pre-computed numerical solutions, are employed to efficiently predict species concentrations and fluxes. Data preprocessing techniques, such as smoothing and feature scaling, further enhance the quality of the predictions. These AI models serve as surrogates for traditional numerical methods, providing a more efficient solution, particularly in cases where chemical reaction calculations dominate computational resources.

The performance of the proposed framework is validated through comparisons with conventional numerical methods, considering various chemical species and heterogeneous porous media. Results demonstrate substantial reductions in computational time while maintaining high accuracy. This approach underscores the potential of AI to accelerate and optimize reactive transport modeling, offering scalable and reliable predictions for applications in environmental management, groundwater contamination, carbon sequestration, and soil remediation.

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MS05 / 551

Application of Packed Bed Reactors and Microfluidic Devices to Simulate Multiscale Bacterial Transport Through a Contaminated Aquifer

Author: James Marquis¹

Co-authors: KaeLee Massey¹; Jinwoo Im²; Michelle Newcomer²; Heidi Smith¹; Yaofa Li³; Al Cunningham⁴; Matthew Fields¹

¹ Montana State University

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Subsurface microbial communities play critical roles in the attenuation of anthropogenic contaminants, as well as global biogeochemical cycling [1]. It has been established that physiological state (whether the organism is sediment-attached or planktonic) may drastically affect metabolic activity levels and rate of bio-degradation [2]. However, due to inherent sampling challenges, accurate prediction of distribution and partitioning of microbial communities within the subsurface remains largely unresolved. Therefore, to determine the empirical relationships between individual microbial cells, growth, attachment, and detachment in a contaminated aquifer requires a laboratory-based approach guided by field observations.

The overarching goal of this work is to disentangle these relationships in the context of the highly contaminated Bear Creek Aquifer, located in Oak Ridge Tennessee. To accomplish this, two reactor systems that mimic the hydrology at different scales were used to simulate subsurface transport conditions and study the transport of the Gram-negative field isolate *Stenotrophomonas GW821-FHT01H02* (*H02*) - a ubiquitous bacterium that is observed in both groundwater and sediments. Packed Bed Reactors (PBRs) were used to simulate the mesoscale; a primary advantage of these systems is the ability to accurately recapitulate much of the spatial and structural heterogeneity of the field. PBRs were packed with sand representing the approximate particle size distribution (75 to 300 μm , $\bar{x}$ = 150 μm) and porosity (ϕ = 0.42) of sediments from the field site. PBRs were inoculated with a pulse of *H02* and operated at two flow rates representing the upper and lower bounds of observed seepage velocities in the field. Results suggested that the partitioning of *H02* is highly sensitive to changes in flow. Under non-growth static conditions, $94 \pm 4\%$ of *H02* cells, regardless of inoculation density, bound to sand particles in the tested size range. This is compared to $55 \pm 3\%$ under the low flow condition and $20 \pm 8\%$ under the high flow condition in the PBRs. Additionally, breakthrough curves of both *H02* and inert tracer bromide (Br^-) were compared at both flow rates. Under both conditions, there was no appreciable difference in time to peak between *H02* and Br^- . However, observational challenges associated with mesoscale reactors made it difficult to distinguish between the effects of microbial growth and attachment kinetics throughout these experiments.

To observe the attachment and detachment processes in real-time while minimizing the effects of microbial growth, we have developed complementary silica oxide microfluidic devices. These devices were intentionally designed to simulate the porosity, mean particle size, and surface properties of the PBRs. Similarly, we have successfully inserted a fluorescent transposon into the genome of *H02* to enable improved visualization and quantification of cells over short-time frames without the use of fluorescent dyes. Initial results indicate that attachment rates of *H02* are highly sensitive to changes in seepage velocity and indifferent to changes in bacterial cell concentration. Furthermore, information regarding attachment and detachment rates gleaned from microscale experiments may improve our ability to predict transport times at larger scales where it is challenging to distinguish between the effects of growth and attachment kinetics.

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Water & Porous Media Focused Abstracts:

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References:

- [1](#) H. J. Smith et al., "Impact of hydrologic boundaries on microbial planktonic and biofilm communities in shallow terrestrial subsurface environments," *FEMS Microbiol Ecol*, vol. 94, no. 12, Dec. 2018, doi: 10.1093/femsec/fiy191. [2](#) V. C. Reyes, S. O. Opot, and S. Mahendra, "Planktonic and biofilm-grown nitrogen-cycling bacteria exhibit different susceptibilities to copper nanoparticles," *Environ Toxicol Chem*, vol. 34, no. 4, pp. 887–897, Apr. 2015, doi: 10.1002/etc.2867.

MS22 / 552

Detecting condensed water in hydrophobic porous media using inverse gas chromatography

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The relevance of dropwise water condensation in hydrophobic media is evident in applications ranging from water harvesting to energy [1](#). However, the physics of water nucleation on hydrophobic substrates (e.g. the impact of structural characteristics versus energetic variability of the surface) is still poorly understood [2](#). The reason is lack of experimental tools sensitive to the small amounts of water nucleating at these surfaces before run-off. In this study, we present a novel technique to detect the nucleation point of water in PTFE samples using inverse gas chromatography (iGC).

iGC is a technique for characterizing the physicochemical properties of porous substrates such as BET surface area and surface energy distribution [3]. In iGC a range of gas probes with known chemical properties, are injected into a column packed with the porous sample under investigation. The probe molecules pass through the column and interact with the porous material. The retention time of the probe molecules is then measured using a flame ionization detector. The variation of retentions measured for probe pulses of systematically varied properties, e.g. concentration and polarity, enables us to determine the physicochemical parameters of the internal surface of the investigated material. Recent advances in commercial IGC enable users to perform the iGC measurements at different controlled humidity [4].

We find that condensed water on the surface of the porous substrate at a given relative humidity impacts the retention of the probe molecules passing through the column during the iGC measurement. We demonstrate that the nucleation point can be detected more accurately with iGC compared to other techniques such as gravimetric dynamic vapour sorption: The reason is the large amount of liquid-gas surface area, the iGC is more sensitive to, with respect to liquid volume generated during condensation in the porous medium. We further demonstrate that the nucleation can be linked to structural properties of the material through the Young Laplace equation. These results provide new avenues to research capillary condensation in hydrophobic systems and aid material development for the mentioned applications.

Country:

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

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554

Effect of Rock Cleaning Process on Acid-Carbonate Reactivity

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The interaction of acidic fluids with carbonate rock formations is a key factor during reactive flow in carbonate acidizing operations. Although several studies have evaluated the reactivity of carbonate rocks, a critical gap remains concerning the influence of pre-experimental cleaning processes. Most studies involving outcrop rocks tend to overlook this aspect, yet the cleaning process can profoundly alter the surface characteristics of the rock, potentially leading to diverse and experimental results without reproducibility. Thus, understanding the impact of these cleaning protocols is essential for accurately interpreting the reactivity results and optimizing acid stimulation strategies.

This study investigates the effect of cleaning processes on the dissolution kinetics of Calcite and Dolomite through static dissolution using miniplugs. Two different permeability ranges were analyzed: low permeability (close to 2 mD) and high permeability (close to 100 mD). The cleaning methods used were based on hot Soxhlet extraction using nonpolar solvents according to API RP 40 standards: (i) toluene/acetone (TA); and (ii) chloroform (Ch). Therefore, three types of cleaning methods were considered: TA, Ch, and no-cleaning.

Miniplugs of 0.80 cm diameter and 1.0 cm length were prepared from larger cores, cleaned, and subsequently dissolved in HCl (1 M) under room conditions. The dissolution rate was quantified by the t₅₀ parameter –the time required for 50% mass loss. The dissolution was verified in four time steps based on the t₅₀: 1/4 of t₅₀, 1/2 of t₅₀, 3/4 of t₅₀, and t₅₀.

The results showed significant differences in the values of t₅₀ and the concentrations of calcium ions –[Ca²⁺]– in the solution for both types of permeability and cleaning protocols. For Calcite samples, the non-cleaning and cleaned samples exhibited similar dissolution behaviors, suggesting a minimal impact of organic residues on acid-rock interactions. In contrast, Dolomite samples showed distinct dissolution trends, indicating that cleaning processes may influence the connectivity of the pore networks and reaction pathways. Moreover, the chloroform methodology revealed a greater increase in the acid dissolution for Dolomite. Micro-CT imaging provided detailed insights into the evolution of pore structures before and after dissolution. For both permeability groups, structural heterogeneities highlighted differences in reaction mechanisms and dissolution efficiency under varying cleaning conditions.

This study contributes to the broader understanding of cleaning-induced alterations in carbonate dissolution kinetics and their implications for subsurface applications. Future work will extend these findings to other carbonate lithologies and consider the influence of higher temperature and pressure conditions.

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556

Visualization of Pore-Scale Reactive Flow Dynamics in Carbonate Rocks Using Synchrotron Radiation (MOGNO Beamline)

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Co-authors: Paulo de Tarso Vieira e Rosa²; Nathaly Lopes Archilha³; Everton Lucas de Oliveira³; Daniel Nobre Nunes da Silva¹; Pedro Tupã Pandava Aum¹

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Reactive flow interactions in porous media are of great relevance in carbonate acidizing operations and in the geological storage of CO₂ and hydrogen. The literature presents advances in understanding certain parameters on the core scale; however, there are still new challenges on the pore scale that can aid in comprehending the phenomenon of acidification. In addition, new discoveries regarding the evolution of the reactive process enhance the modeling of geological storage applications. Therefore, the objective of this work is to present the temporal evolution of the available rock surface area during reactive flow in porous media. The study was carried out on limestone and silurian dolomite rock samples from Indiana with dimensions of 2.5×2.5 mm in diameter and length, respectively, and 0.1 M HCl was used as the acid agent in reactive flow experiments. The analyses were performed at the MOGNO beamline of the Brazilian Synchrotron Light Laboratory, where a fluid flow cell was developed to allow time-resolved image acquisition during fluid flow in the sample. The MOGNO beamline X-ray microtomography technique, which utilizes synchrotron light as an energy source, was used to visualize the interior of the sample. The injection of acid was performed at a flow rate of 10 µL/min for 1 hour, during which 7 scans were acquired with a resolution of 1.2 µm. Our findings reveal the dynamic temporal evolution of the surface area parameters available for reaction and porosity during the reactive flow in each sample at the pore scale. The evolution of these parameters is more evident in the Indiana Limestone sample as a result of the faster reaction rate with this type of mineralogy. In conclusion, these findings contribute to advance the understanding of reactive processes in porous media and provide data to improve models for geological storage applications.

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MS03 / 557

Numerical simulation of Krauklis wave propagation in complex 2D fracture systems

Author: Seiji Nakagawa¹

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Corresponding Author: snakagawa@lbl.gov

Recently, Krauklis waves (Krauklis, 1962)—guided waves that propagate mostly as pressure pulses within fluid-filled, high-permeability fractures—have gained attention as a geophysical tool for sub-surface fracture characterization. Strongly dispersive velocity and attenuation of these waves are sensitive to the hydraulic conductivity (permeability) of the fractures. This property may give Krauklis waves advantages over other types of fracture guided waves and body waves for probing the connectivity of the fracture, because the latter are sensitive to the local permeability of the fractures (via local fracture compliance) that may not reflect the actual reservoir permeability. However, fractures in rock exist at many scales, forming a complex network including microcracks within the rock matrix. In such a system, Krauklis waves can be quickly scattered, attenuated, and converted to body waves. In this research, the behavior of Krauklis waves in a variety of complex fracture systems is examined, using a 2D time-harmonic boundary element method. The local interactions between fluid-filled compliant fractures and the rock matrix are modeled via a poroelastic linear-slip interface (seismic displacement-discontinuity boundary) model, which allows efficient computation of the complex interactions between the waves and the fractures (Nakagawa, 2024).

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Water & Porous Media Focused Abstracts:

References:

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MS23 / 558

Competitive Sorption of CO₂ and H₂ on Coals: Implication for Simultaneous H₂ Cleaning and CO₂ Storage in Depleted Coalbed Methane Reservoirs

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The imperative shift towards a decarbonized hydrogen economy necessitates a transition from the current reliance on unabated fossil fuel-based hydrogen production, which results in significant CO₂ emissions. This study proposes a novel approach to address this challenge by introducing a groundbreaking concept for the simultaneous separation of hydrogen (H₂) and permanent storage of carbon dioxide (CO₂) within depleted coalbed methane (CBM) reservoirs. This study investigates CO₂-H₂ competitive sorption in sub-bituminous and anthracite coals, addressing experimental challenges and model limitations. The experimental sequence included initial sorption tests with pure CO₂ and H₂ gases, followed by adsorption of the pre-mixed CO₂-H₂ mixture and the subsequent desorption after each adsorption equilibrium. Higher pure CO₂ adsorption compared to pure H₂ adsorption has been observed. In pre-mixed CO₂/H₂ adsorption, the mixture gas adsorption isotherms confirm the competitive sorption nature of CO₂-H₂ in coals. These isotherms demonstrate that gas adsorption is generally lower for binary gas injection compared to their pure gas counterparts, with the effect increasing as fugacity and molar fraction of the second gas rise. Subsequent desorption of CO₂/H₂ mixtures under varied conditions reveals competitive sorption effects of CO₂ over H₂, leading to higher sorbed amounts of CO₂ and lower sorbed amounts of H₂, consistent with observed composition ratio changes. Solubility-selectivity analysis elucidates coal-dependent trends in CO₂/H₂ competitive sorption. The study emphasizes the significant impact of multicomponent scenarios on coal selectivity for CO₂ and H₂, cautioning against sole reliance on pure-gas data for accurate estimations.

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559

Exploring the Influence of the Viscosity Ratio and Fluid Velocity on Dynamic Fluid Connectivity and Rapid Pore-Filling Events

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Co-authors: Amir Jahanbakhsh¹; M. Mercedes Maroto-Valer¹

¹ Heriot-Watt University

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Understanding the fundamentals of immiscible two-phase fluid displacement in porous media is crucial for applications like groundwater remediation, CO₂ sequestration, and enhanced oil recovery (EOR) (1). Key processes, such as drainage and imbibition, are affected by fluid viscosity, density, interfacial tension, and the porous media's wettability (2).

In CO₂ sequestration, for example, interfacial instabilities, like viscous and capillary fingering, complicate the drainage processes, while Haines jumps can affect CO₂ stability and mobility (3). Understanding these pore-scale instabilities is crucial for assessing injectivity, mobility, and saturation, which impact storage capacity and leakage risks (2). Numerical simulations are vital for comprehending such complex multiphase flow dynamics and developing models for larger spatial scales (4).

This study aims to enhance the understanding of the complex interfacial dynamics involved in two-phase displacement processes. To achieve this, direct numerical simulations in OpenFOAM were conducted using a Berea sandstone model to investigate how fluid viscosity and velocity influence pore-filling events during immiscible two-phase fluid displacement.

The movement of two proxy fluids—water and decane—within the porous Berea sandstone matrix was analysed, as they differ in viscosity. In this context, water acted as the displacing fluid while decane served as the displaced fluid. In all simulations, the viscosity of water was maintained at 1 cSt, while the viscosity of the decane phase varied between 0.0125 cSt and 125 cSt, resulting in a two-phase system mobility ratio (M) where $-2 \leq \text{Log } M \leq 2$. To eliminate wettability effects, the sandstone was treated as neutral-wetted, with a contact angle of 90° . The study explored a capillary number range of $-3 \leq \text{Log } Ca \leq 1$.

Results showed a transition from connected pathway flow (CPF) to droplet traffic flow (DTF) as the invading fluid velocity increased, leading to reduced fluid connectivity at higher capillary numbers. At $\text{Log } Ca = -1$ and -2 , the fluid front moved only forward, but at $\text{Log } Ca = -3$, both forward and backward movement (Figure 1) occurred due to Haines jumps.

These jumps induced rapid fluid front acceleration and fluctuations in pressure and saturation, altering fluid configurations. Local dynamics during these events decoupled from the average flow rate, resulting in local pressures and velocities significantly higher than the imposed average.

The frequency of Haines jumps decreased with increasing viscosity of the invading phase, transitioning from $\text{Log } M = 1$ to $\text{Log } M = -2$. Despite decreased frequency, the volume of these jumps (ΔV) increased from 4% to 43%, with an average timescale extending from 12 to 50 milliseconds. These jumps were correlated to meniscus retraction and snap-off events, influenced by local and global dynamics. Notably, the magnitude of pressure pulses was inversely related to the jump's zone of influence.

Overall, these findings suggest that pore drainage events are non-local processes influenced by the spatial arrangement of bulk fluids, affecting drainage rates and macroscopic displacement fronts. Haines jumps may complicate CO₂ sequestration and enhanced oil recovery processes, especially when coupled with distal snap-off events that render portions of the porous matrix inaccessible.

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An immobilized hybrid adsorbent / photocatalyst system: ZnO nanoparticles on 3D porous graphene

Authors: Athanasios Souliotis¹; Nikolaos Samartzis¹; Spyros N. Yannopoulos¹

Co-authors: Kapil Bhorkar ¹; Labrini Syggelou ¹

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The remediation of polluted water remains a critical environmental challenge due to the increasing anthropogenic activity. Advanced materials offer promising solutions for wastewater treatment by enabling contaminant adsorption and catalytic degradation [1]. Among these, nanostructured carbon materials, such as 3D porous graphene, exhibit high potential due to their high surface area, tunable porosity, and modifiable surface chemistry [2].

In this study, we introduce a novel, scalable, and eco-friendly method for synthesizing 3D porous graphene decorated by ZnO nanoparticles to address water pollution. Using the Laser-assisted Explosive Synthesis and Transfer (LEST) technique, porous graphene-like films were deposited onto metallic Zn foil substrates [3]. Upon immersion in aqueous solutions, the graphene films underwent in-situ decoration with ZnO microflowers, a process that occurs spontaneously under ambient conditions.

The resulting graphene/ZnO hybrid material exhibits a dual function for pollutant removal: (i) high adsorption efficiency due to the π - π interactions of sp^2 carbon with aromatic molecules and (ii) effective photocatalytic degradation under UV light, facilitated by the ZnO microstructures. Photocatalytic experiments using methylene blue (MB), a model cationic dye pollutant, demonstrate that the material achieves significant pollutant removal through combined adsorption and photocatalysis. The photocatalytic performance remains stable over multiple cycles, demonstrating the material's reusability. Specifically, after a few photocatalytic cycles, the degradation rate remained approximately 80% after 25 hours, which is higher than the rate achieved using a film of ZnO nanoparticles as a photocatalyst without the 3D porous graphene substrate.

The observed pollutant degradation was correlated with the properties of the graphene/ZnO nanohybrids using various characterization techniques. The porous network observed through scanning electron microscopy (SEM) is characteristic of graphene-like structures synthesized via laser irradiation. This network is attributed to the rapid release of gases formed during the thermal decomposition of the carbonaceous precursor, induced by the absorption of laser pulses [4]. Raman and photoluminescence spectroscopies, along with X-ray photoelectron spectroscopy, revealed the time-dependent evolution of ZnO nanoparticles upon immersing the Zn-supported LEST-graphene films in water.

The LEST-based synthesis method offers significant advantages, including low energy consumption and compatibility with various substrates, making it a sustainable approach for producing advanced 3D porous materials. This study highlights the potential of 3D porous graphene/ZnO hybrids as multifunctional materials for wastewater treatment and lays the groundwork for further exploration of in-situ decoration strategies for environmental applications.

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1 M. Lewoyehu, Comprehensive review on synthesis and application of activated carbon from agricultural residues for the remediation of venomous pollutants in wastewater, *J. Anal. Appl. Pyrolysis* 159 (2021) 105279. <https://doi.org/10.1016/j.jaap.2021.105279>. **2** K. Gu, E.J. Kim, S.K. Sharma, P.R. Sharma, S. Bliznakov, B.S. Hsiao, M.H. Rafailovich, Mesoporous carbon aerogel with tunable porosity as the catalyst support for enhanced proton-exchange membrane fuel cell performance, *Mater. Today Energy* 19 (2021) 100560. <https://doi.org/10.1016/j.mtener.2020.100560>. [3] K. Bhorkar, N. Samartzis, M. Athanasiou, L. Sygellou, N. Boukos, V. Dracopoulos, T. Ioannides, S.N. Yannopoulos, Laser-assisted explosive synthesis and transfer of turbostratic graphene-related materials for energy conversion applications, *Npj 2D Mater. Appl.* 6 (2022) 56. <https://doi.org/10.1038/s41699-022-00331-7>. [4] N. Samartzis, M. Athanasiou, V. Dracopoulos, S.N. Yannopoulos, T. Ioannides, Laser-assisted transformation of a phenol-based resin to high quality graphene-like powder for supercapacitor applications, *Chem. Eng. J.* 430 (2022) 133179. <https://doi.org/10.1016/j.cej.2021.133179>.

Poster / 561

Investigation of the impact of microbial activity and biofilm formation on multiphase flow in porous media using X-ray micro-CT.

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Biofilms are living, highly dynamic, microbial communities embedded in a matrix of secreted extracellular polymeric substances (EPS). These complex microbial communities have a significant impact on the petrophysical properties of porous media that they colonise (Jin & Sengupta, 2024). This leads to changes in pore geometry, tortuosity, porosity, wettability, capillary pressure and saturation which, in the context of underground hydrogen storage, can lead to hydrogen trapping and reduced recovery during cyclic injection (Pasca et al., 2015; Jangda et al., 2022; Raza et al., 2022).

This interdisciplinary project employs anaerobic and selective culturing techniques to effectively grow and cultivate relevant biofilm forming isolates. Batch experiments run under representative reservoir conditions with relevant strains and enrichment cultures will provide a time-resolved look at gas consumption and microbial activity over time. X-ray micro-CT imaging will be utilised to look inside inoculated cores without destroying them. Digital analysis of the scanned cores will allow for the observation of changes in multiphase flow in these rock-hydrogen-brine-biofilm systems and determine what impact biofilms could have on hydrogen recovery.

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Pasca et al., 2015; Jangda et al., 2022; Raza et al., 2022; Jin & Sengupta, 2024

MS08 / 562

Enhanced Mixing in Porous Media Through Electroosmotic Flow

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Mixing in porous media and microfluidic devices can play a crucial role in various processes, including in-situ mining of minerals, geothermal heat extraction, and efficient operation of microreactors. However, such environments typically support flow at low Reynold's numbers, so achieving controllable mixing can be challenging. To address this, electric fields can offer an externally adjustable way to enhance mixing through electrokinetic flow. We explore the interaction between electroosmotic and pressure-driven flows in heterogeneous porous media through experiments using Hele-Shaw cells. Specifically, we focus on the relationship between cell heterogeneity, flow recirculation, and mixing. When a charged surface comes into contact with an electrolyte solution, a diffuse layer of counter-ions forms, creating the electric double layer that screens the surface charge. Applying an external electric field parallel to the solid surface induces electroosmotic flow via an effective slip at the solid surface. In regions of high permeability, pressure-driven flow dominates, whereas, in narrow spaces, electroosmotic flow prevails, leading to recirculating flows between high- and low-permeability zones. By harnessing the interaction between these two flow mechanisms, we characterize electroosmotic mixing in porous media.

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MS26 / 563

Small heterogeneities with large impacts on CO₂ flow and trapping

Author: Sam Krevor^{None}

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In this presentation I will argue that small, centimetre scale, heterogeneities in multiphase flow properties will have field scale impacts on the movement of CO₂ injected underground. I will demonstrate our characterisation and modelling workflows in application to simulations of CO₂ storage sites of the offshore UK (An et al., 2023; Wenck et al., 2025). In search of a validating case study, my research

group has been reinterpreting seismic imagery from the Decatur CO₂ storage site in the USA (Bukar et al., 2025). I will show results of our application of an interpretation of the time-shifts from seismic surveys at this site. This has revealed CO₂ migration along faults, allowing the plume to bypass lower quality units within the reservoir.

An, S., Wenck, N., Manoorkar, S., Berg, S., Taberner, C., Pini, R., & Krevor, S. (2023). Inverse modeling of core flood experiments for predictive models of sandstone and carbonate rocks. *Water Resources Research*, 59(12), e2023WR035526

Bukar, I., Bell, R. E., Muggeridge, A., & Krevor, S. (2025). Carbon dioxide migration along faults at the Illinois Basin–Decatur Project revealed using time shift analysis of seismic monitoring data. *Geophysical Research Letters*, in Press

Wenck, N., Muggeridge, A. H., Jackson, S. J., An, S., & Krevor, S. (2025). The Impact of Capillary Heterogeneity on CO₂ plume migration at the Endurance CO₂ storage Site in the UK. *Geoenery*, in Press

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MS15 / 564

Upscaling Microscale Flow Effects using Differentiable Programming

Authors: Agnese Marcato¹; Daniel O'Malley^{None}; Eric Guiltinan¹; Hari Viswanathan¹; Javier E. Santos²

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Accurately predicting fluid flow through fractured media remains a major challenge due to the disparity between simple modeling assumptions and the complex reality of fracture geometry. Fractures at the continuum-scale are represented as very simple geometries, but in reality, fractures are quite complex. Assuming a parallel plate-like geometry in our numerical models can yield very high errors for fluid transport. While there have been numerous attempts to come up with a relationship that conveys micro-scale information about how fracture geometry influences flow at the continuum-scale, a universal equation remains elusive. This is partly due to the fact that effective properties used in these relationships fail to capture enough of the complexity of real fracture geometries. Machine learning approaches are promising, but integrating flow physics as hard-constraints in architectures has not been possible. Here, we introduce a novel application of differentiable programming in geosciences, enabling data-driven learning that adheres to fundamental conservation laws. This novel approach connects micro- and continuum-scale behavior, allowing us to come up with a general model for the permeability of rough, complex fractures. Our work paves the way for significantly improved flow predictions and ultimately a deeper understanding of multi-scale flow dynamics.

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References:

Poster / 565

X-Ray Microtomography for Evaluating Groundwater in-situ Chemical Remediation at Pore-Scale

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In situ chemical oxidation (ISCO) has become a widely used remediation technique for contaminated areas due to its proven effectiveness. The use of potassium permanganate (KMnO₄) to degrade trichloroethylene (TCE, C₂HCl₃) has demonstrated favorable results in both pilot- and field-scale studies. However, a key challenge in optimizing the process lies in the limited understanding of reactions at the microscale.

This work seeks to investigate the pore-scale dynamics of the ISCO remediation process of TCE using KMnO₄. The study employs 3D synchrotron-based computed microtomography (μCT) to capture time-resolved images of an injection experiment conducted in a porous medium. Initial characterization of the water-saturated sample provided crucial data, including total porosity, grain surface area, and pore tortuosity. Analysis of samples saturated with TCE and KMnO₄ revealed changes in permeability, residual contaminant levels, and the formation of reaction products.

Country:

Brasil

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Water & Porous Media Focused Abstracts:

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References:

MS19 / 566

Upscaling of lithium-ion battery models: from the pore-scale to the cell-scale through homogenization

Author: Alessio Lombardo Pontillo¹

Co-authors: Agnese Marcato²; Daniele Marchisio¹; Gianluca Boccardo¹; Ilenia Battiatto³

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Lithium-ion batteries (LiBs) are currently the leading energy storage technology for applications ranging from portable devices to aerospace vehicles. They are also expected to play a significant role in net-zero energy buildings, with global battery demand projected to increase by approximately 27% annually until 2030. Their advantages include a high energy-to-weight ratio, low self-discharge, and decreasing production costs, making them a top choice for future non-fossil fuel-powered systems [1](#). However, improving LiB performance and lifetime requires addressing challenges such as non-uniform current distribution, which is strongly influenced by electrode morphology.

Graphite, the most commonly used material for anodes, has a flake-like anisotropic structure due to its hexagonal atomic arrangement. This geometry is crucial to the electrochemical processes in LiBs but is often oversimplified in models, which typically assume spherical particles. While this approximation may suffice for cathodes, it fails to capture the complex behavior of graphite anodes, leading to inaccuracies in performance predictions. Therefore, accurately reconstructing the microscopic geometry of the electrode is vital for understanding charge and discharge processes on a macroscopic scale [2](#).

This study focuses on the geometrical characterization of graphite electrodes in a half-cell setup. The goal is to develop an upscaled model using homogenization techniques, enabling faster and more computationally efficient simulations. The team began by identifying a particle shape that balances realism and computational cost. An ellipsoidal shape was chosen, with two larger dimensions derived from particle size distribution (PSD) data and aspect ratios evaluated from scanning electron microscope (SEM) images. This approach provides a more realistic representation of graphite particles compared to spherical approximations, as confirmed by experimental porosity evaluations.

The electrode geometry was created through a semi-automated process using Python-based tools. Initially, the software Yade-DEM was used to generate a packing of spheres based on PSD data. These spheres were then transformed into flattened ellipsoids using Blender, and a rigid-body simulation compacted the layer to reduce voids. The central portion of the packed layer was extracted and used as input for pore-scale simulations in COMSOL 6.1. This Python-controlled workflow allows the creation of various electrode morphologies and particle size distributions.

Homogenization techniques were applied to derive macroscopic properties from microscopic behavior. This involved rewriting equations in dimensionless form to extract parameters like the Damköhler and Péclet numbers, which determine the feasibility of scale separation. A closure problem was solved on a periodic unit cell, containing polydisperse ellipsoids and semi-ellipsoids, to calculate effective diffusivity and conductivity values for the solid and liquid phases [3-4]. These effective properties were then used to create and solve a homogenized model.

The homogenized model produced results comparable to those of the computationally intensive pore-scale simulations but required significantly less time and resources. The flexible script enables the generation of diverse electrode geometries, facilitating the creation of a large dataset across a wide parameter space. This dataset could be used to train neural network models, offering a quick surrogate method to explore various electrode configurations. This approach represents a significant step toward optimizing LiB design and performance.

Country:

Italy

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Water & Porous Media Focused Abstracts:**References:**

[1] McKinsey & Company, (2023), Battery 2030: Resilient, sustainable, and circular, <https://www.mckinsey.com/industries/automotive-and-assembly/our-insights/battery-2030-resilient-sustainable-and-circular> [2] Lu, X., Lagnoni, M., Bertei, A. et al., (2023), Multiscale dynamics of charging and plating in graphite electrodes coupling operando microscopy and phase-field modelling. *Nat Commun* 14, 5127. [3] Arunachalam, H., Onori, S., Battiatto, I., (2015), On Veracity of Macroscopic Lithium-Ion Battery Models. *J. Electrochem. Soc.*, 162, A1940. [4] Battiatto, I., Tratakovsky, D.M., (2011), Applicability regimes for macroscopic models of reactive transport in porous media, *J. Contaminant Hydrology*, 120-121, 18-26.

MS10 / 568

Time resolved spectral micro-CT imaging: monitoring compositional changes during dissolution

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Micro-CT is a unique technology to non-destructively investigate the internal structure of geological samples, spanning a range from centimeter to micrometer scale. The non-destructive nature makes the technique ideal for studying dynamic processes, allowing to visualize geological material behavior when exposed to external conditions like temperature, pressure or to certain fluids. Time resolved or dynamic micro-CT has been applied in a wide variety of fluid flow studies, providing valuable information on pore scale fluid dynamics. Especially when investigating reactive fluid flow in complex geological materials, time resolved micro-CT imaging can provide valuable information inside the sample, as it can pinpoint where chemical reactions are occurring in the pore space and which minerals are associated with these reactions.

In order to locally pinpoint compositional changes in the fluid or associated minerals inside a geological material, conventional micro-CT 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 mainly by its atomic number and density, but also other parameters like X-ray energy, the X-ray spectrum, and the characteristics of the employed detector can play a role. With all these factors collectively contributing to the observed contrast, extracting compositional and density information from conventional micro-CT data, can be a challenging endeavor.

In this research, a new and emerging technique called spectral X-ray computed micro-tomography (spectral CT) is used in combination with time resolved imaging to obtain better insights in leaching processes and extract compositional changes in 3D throughout the leaching process. Spectral CT is used to monitor local compositional changes in grain pack while a leaching solution (acid) is pumped through the grain pack. By utilizing a spectral detector, providing attenuation information for each energy in the X-ray spectrum, a more precise quantification of mineralogical changes in the grain pack and the compositional changes in the leaching fluid in the pore space can be obtained. In this work we will illustrate how time resolved spectral micro-CT can be utilized to improve our understanding of complex reactive fluid flow processes.

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Water & Porous Media Focused Abstracts:**References:**

Poster / 569

Experimental study on permeability evolution due to salt crystallization at the REV scale

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Salt Crystallization in Porous Media is a critical phenomenon found in various natural processes and applications, such as the degradation of built structures, gas recovery and storage, and underground CO₂ storage. This phenomenon impacts the petrophysical properties of rocks, particularly porosity and permeability, fundamental parameters in the description of fluid flow in porous media. The reduction of permeability due to salt crystallization is typically estimated in reservoir simulators by means of empirical relationships. However, the validity of these relationship is not always guaranteed, and precise experimental data on the link between salt crystallization and permeability is scarce.

We developed an experimental protocol promoting, as much as possible, a homogeneous distribution of salt crystals at the scale of the representative elementary volume (REV), enabling a reliable assessment of their impact on permeability. We therefore propose an experimental approach based on vacuum drying. We conducted successive cycles of saturation with a potassium chloride saline solution, followed by vacuum drying, on various artificial porous media samples with different pore sizes (VitraPOR cylinders, 6 mm diameter, pore sizes between 40-100 µm, 100-160 µm, 160-250 µm, 250-500 µm). These cycles were repeated until a maximum amount of salt was reached within the porous medium. At each step, X-ray tomography scans were performed to quantify and visualize salt deposits, alongside weight measurements to compare the amounts of precipitated salt. After each cycle, the permeability was measured experimentally by placing the confined sample in a Hassler cell and measuring the pressure drop over the sample while injecting an inert fluid at a controlled rate.

The results of this study demonstrate that vacuum drying allows for a homogeneous distribution of salt crystals within the pore network, with a progressive accumulation of salt after each cycle as precipitation primarily remains in the same locations (Figure 1). Such homogeneity was not achieved using conventional drying methods, which tend to induce heterogeneous crystallization, primarily at the sample edges, making it difficult to establish an accurate experimental relationship between permeability and salt quantity. Successive permeability measurements enabled us to establish an experimental curve linking permeability to the deposited salt mass. These findings provide a promising avenue for improving and refining the modeling of physical phenomena involving salt crystallization in porous media. Future perspectives of this study include expanding the experiments to different types of natural rocks, such as Savonnières limestone and Bentheimer sandstone, as well as using a more commonly encountered salt in various application domains where this phenomenon occurs, namely NaCl.

Acknowledgements: The authors acknowledge the support from the ERC Starting Grant PRD-Trigger (grant agreement N° 850853), the Fédération de Recherche IPRA (FR CNRS-UPPA 2952), and the Research Foundation Flanders (FWO, G004820N).

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Student Awards:**Water & Porous Media Focused Abstracts:**

This abstract is related to Water

References:**Poster / 570**

Water and Soil Moisture Impacts on Dust Storm Emissions

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Sand and dust storms (SDS) and emissions are extreme weather events that can silently cross borders and impact millions globally. The SDS can pose threats to environmental and human health across all continents. These storms arise from complex interactions between atmospheric and land factors, with soil properties playing a pivotal role in their formation, intensity and consequence impacts. Soil, as a porous medium, governs the mobilization of SDS particles by wind, and its moisture content is a critical element in reducing erosion caused by winds. Soil moisture binds particles together, thereby reducing the likelihood of SDS events. On the other hand, dry and degraded soils become more vulnerable to wind erosion, increasing the frequency and intensity of SDS. Recognizing the importance of mitigating SDS events and impacts, the United Nations has declared 2025–2034 as the Decade on Combating Sand and Dust Storms.

Among various sources of data for monitoring SDS, NASA's Atmospheric Infrared Sounder (AIRS) satellite provides valuable global-scale, daily observations of dust storm location and intensity. In this study, we analyze more than 47 terabytes of AIRS data spanning a 22-year period to identify spatiotemporal trends in dust storms at a global scale. This dataset comprises approximately 2 million HDF files, each with an average size of 25 MB. By employing a parallel computing scheme, we process these extensive datasets efficiently to estimate the global evolution of dust storm activity over time.

Our findings reveal a strong correlation between decreasing water equivalent height (WEH), decreasing soil moisture levels and the increasing occurrence of dust storms. Specifically, regions exhibiting more negative values in WEH are becoming significant sources of dust emissions. This indicates that water availability in the soil plays a crucial role in suppressing dust storms. Additionally, our study highlights the potential of satellite-based observations in providing actionable insights into SDS dynamics, contributing to more effective mitigation strategies. Understanding the interplay between soil moisture, land degradation, and dust storm emissions is essential for developing adaptive measures to reduce the environmental and societal impacts of these transboundary phenomena.

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Student Awards:**Water & Porous Media Focused Abstracts:**

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References:

MS06-A / 571

Quantifying Threshold Capillary Pressure in Sedimentary Matrix-Lamina Bedding Pairs using Pore-Scale Simulation

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In multiphase flows near capillary equilibrium, such as the buoyant migration of fluids in the subsurface, small changes in the capillary pressure can play important roles in the dynamics of such systems. Capillary pressure variations are controlling factors for the migratory pathways of fluids such as those in petroleum, natural gas, geologic carbon sequestration, and geologic hydrogen storage. Typically, rock-fluid injection tests, such as core flooding, are used to characterize the capillary pressure behavior of rocks to be used for further analysis. In their absence, very generalized empirical approximations are used to estimate different capillary pressures of rocks. However, these simple approximations are only valid within certain assumptions originally formulated for unconsolidated sphere packings or soils.

When considering frequent and distinct variations in pore morphology, as in highly laminated geology, small variations of pore size distribution may not be adequately considered in capillary pressure approximations. Singular measures of average porosity, permeability, and/or pore size ignore potentially multimodal properties of rocks such as the capillary pressure of a contrasting lamina within a sedimentary rock matrix.

To study this, simplified, digital geometries containing regions of contrasting circle size distribution are generated to replicate a lamination in sedimentary rocks. Flow perpendicular to the layering is simulated using a lattice Boltzmann color gradient method for multiphase flow. CO₂ drainage is simulated until breakthrough to the opposite side, and the time-variant saturation of the domains and regions, as well as the CO₂ phase pressure, is calculated for various contrasts.

While the circle sizes, or grain sizes, of the fine-grained region are seen to be a dominant property for threshold capillary pressures, the capillary pressure curves may be influenced by the pattern matrix geometry; as such, descriptions of the influence of the matrix-lamina contrast are also discussed. Further, these sorts of findings attempt to show underlying patterns that could be used to estimate the capillary pressure characteristics of laminated architectures given some pore-level characteristics.

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United States of America

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Water & Porous Media Focused Abstracts:

References:

MS26 / 572

Using changes in soil moisture to detect CO₂ leakage in real-time

Authors: Aria Chavoshi Boroujeni¹; Hassan Dashtian¹; Mahdi Haddad¹; Sahar Bakhshian²

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One of the key issues related to geologic CO₂ storage is the risk of leakage of both CO₂ and brine to the surface. Wellbores are usually the main conduit of CO₂ leakage. Legacy wells, often remnants of previous oil and gas operations, are particularly problematic because they are abundant in areas targeted for CO₂ storage and may fall within the area of review. These wells, if not properly completed or plugged, can serve as pathways for fluids to migrate to the surface or into sensitive subsurface zones. This necessitates the constant monitoring and assessment of legacy wells to ensure they are adequately sealed and do not pose a risk of leakage. Consequently, there is an urgent need for robust and efficient monitoring systems capable of providing early detection of CO₂ and brine leakage, which is vital for minimizing both environmental damage and financial repercussions.

Our study aims to address this challenge by designing and implementing a cost-effective near-surface monitoring system that can provide real-time, long-term surveillance of plugged and abandoned (P&A) wells. This system is intended to be both scalable and adaptable, making it suitable for various site conditions and leakage scenarios. To achieve this, we conducted a series of pilot-scale experiments involving controlled releases of CO₂ and brine. These experiments were designed to simulate leakage events under a range of conditions, including varying leakage rates and durations. The primary goal was to identify the most sensitive and reliable parameters for detecting fluid migration into vadose zone.

The experiments revealed that soil electrical conductivity (EC) is the most responsive soil signature to CO₂ and water leakage. This sensitivity makes EC a valuable parameter for near-surface monitoring systems. By combining EC measurements with advanced data analysis techniques, we were able to improve the accuracy and reliability of leakage detection. Specifically, we integrated a Physics-Informed Neural Network (PINN) model with a supervised classification machine learning algorithm to analyze the data. This hybrid approach allowed us to distinguish between anomalies caused by fluid leakage and those resulting from natural environmental variations, such as changes in soil moisture or temperature. The PINN model provided a framework for incorporating physical principles into the analysis, enhancing the model's ability to interpret complex datasets and predict leakage events with high precision.

Furthermore, the system's ability to operate in real-time and provide continuous monitoring is a significant advantage. Real-time data collection and analysis enable rapid response to potential leakage events, reducing the risk of extensive environmental damage. The long-term surveillance capability ensures that P&A wells can be monitored throughout the lifecycle of a CO₂ storage project, providing ongoing assurance of their integrity.

In addition to its technical benefits, the proposed monitoring system is designed to be cost-effective, which is crucial for its widespread adoption in commercial CCS projects. The use of readily available sensors and advanced data processing techniques minimizes operational costs while maximizing efficiency. This makes the system a practical solution for monitoring large numbers of legacy wells, even in resource-constrained settings.

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References:

MS18 / 573

Microplastic Dynamics in Hollow Fiber Membranes: Advanced Fluorescence Detection and Pore Network Transport Modeling

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Microplastic (MP) contamination in aquatic environments continues to present a significant challenge for water treatment and environmental management. These tiny plastic particles, resulting from industrial activities and the breakdown of larger plastics, have been shown to accumulate in natural water systems, posing risks to ecosystems and human health. Understanding how microplastics interact with filtration systems, particularly membranes, is critical to optimizing water treatment technologies and mitigating environmental impacts. This study explores the interactions between microplastics and hollow fiber membrane pore sizes, employing an innovative combination of fluorescence staining dye (MP), detection techniques and transport phenomena modeling through pore network analysis (PNM).

The fluorescence detection method leverages Nile Red (NR) staining, a well-established technique for visualizing microplastics, to directly detect and analyze microplastic particles in aqueous environments. This approach eliminates the need for extensive pre-treatment, offering a streamlined and efficient method for identifying microplastic presence. Hollow fiber micro- and ultrafiltration membranes serve as model systems in this study, providing insight into how pore size distributions influence microplastic retention, transport, and clogging mechanisms under varying operational conditions.

Fluorescence microscopy and spectroscopy are utilized to capture detailed observations of microplastic retention and transport phenomena within the membranes. These experimental findings are further supported by pore network modeling, which simulates the dynamics of microplastic movement, accumulation, and fouling at the microscale. This dual-method approach bridges experimental and computational insights, enabling a comprehensive understanding of microplastic behavior in porous systems.

Initial findings highlight the critical role of membrane pore size, flow velocity, and particle properties in determining retention efficiency and fouling potential. Experimental validations using synthetic and real wastewater matrices demonstrate the robustness of this combined approach in characterizing microplastic dynamics in diverse conditions. Moreover, the results reveal key interactions between microplastics and hollow fiber membrane structures, contributing to the optimization of filtration performance and the design of more efficient water treatment systems.

Looking forward, this research aims to expand its scope to include a wider range of polymer types and membrane geometries, enhancing the resolution of pore network models to predict microplastic behavior more accurately. Future investigations will focus on exploring the long-term impacts of microplastic interactions on membrane fouling, durability, and overall filtration efficiency. Additionally, the potential integration of this approach with advanced monitoring technologies, such as real-time fluorescence sensors, offers promising avenues for further innovation.

By integrating experimental detection with computational modeling, this study establishes a framework for advancing the characterization of microplastic behavior in filtration systems. The findings provide critical insights that can inform the development of tailored solutions for addressing microplastic contamination in water treatment and environmental remediation efforts. This work

underscores the importance of interdisciplinary approaches in tackling complex environmental challenges and highlights the potential for innovative techniques to drive sustainable solutions.

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References:

MS10 / 576

Rocking Fluid Flow: High-Speed X-ray Imaging of Natural Rocks at ESRF

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Co-authors: Joris Heyman²; philippe gouze²; Tanguy Le Borgne³

¹ ESRF

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Understanding fluid dynamics within natural rock formations is crucial for optimising porous fluid flow with direct applications for CO₂ mineral trapping and hydrogen production. At the European Synchrotron Radiation Facility (ESRF), technological advancements have significantly enhanced our ability to observe these phenomena in real time and under in situ conditions.

ESRF's beamline ID19 has been at the forefront of developing ultra-fast X-ray imaging techniques. Notably, high-resolution volumetric imaging enables capturing dynamic processes with remarkable temporal resolution. These methods involve quickly acquiring systems under high Peclet numbers under stationary conditions. Promising advancements now also allow the exploration of non-stationary processes. In addition, ESRF has pioneered megahertz projection imaging capable of recording volumetric information at MHz rates and micrometre resolution without necessitating sample rotation, facilitating the study of rapid, non-reproducible processes in four dimensions (3D + time).

The Block Allocation Group (BAG) initiative CHRONOS, on beamlines BM18 and BM05, extends the value of these imaging techniques by supporting long-term experimental projects. This framework is particularly beneficial for studying CO₂ mineral trapping and hydrogen production under prolonged and natural conditions, providing unprecedented insights into fluid-rock interactions over time.

The combination of ultra-fast imaging techniques and the CHRONOS BAG framework at ESRF offers a powerful platform for advancing our understanding of fluid flow in natural rocks. We encourage exploring the complexities of fluid-rock interactions with the present capabilities and developing them to advance our knowledge in geosciences continually.

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References:

MS16 / 577

Surface washing of contaminated porous substrates

Authors: Georgia Ioannou¹; Francesco Paolo Conto²; Merlin A. Etzold³; Julien R. Landel⁴; Stuart B. Dalziel¹

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The cleaning and decontamination of various porous surfaces (e.g., concrete, tarmac, wood, etc.) is a challenging and multidisciplinary problem for both fundamental understanding and a wide range of industrial, medical, urban, everyday-life and disaster-response applications. The role of such processes is particularly crucial in cases where contaminants, such as chemical substances and biological pathogens, are extremely harmful and pose serious risks to human health. Indeed, attempts to decontaminate porous materials might lead to a partial redistribution of the unwanted substance within the porous matrix instead of a complete removal. As a result, cleaning operations could further contribute to the contaminant/virus spread, and the substance might remain a long-time hazard for people coming in contact with the contaminated medium.

We performed surface-washing experiments modelling the decontamination of porous media. The contaminant agent was simulated by a passive tracer (disodium-fluorescein solution) which was released onto the free porous surface in the form of droplets and was let to diffuse in the porous structure. The surface-washing was simulated by a thin gravity-driven water film flowing over the inclined porous-glass plane. A parametric analysis was conducted by varying parameters such as the amount of the contaminant, the angle of the porous plate with the horizontal, the time from the contaminant deposition on the porous plate until the start of washing, and the permeability of the porous plate. A novel method based on spectroscopy principles was developed to measure precisely the concentration of the contaminant that has been removed from the porous plate and is present in the effluent with time. Additionally, employing imaging techniques we extracted valuable qualitative information about the contaminant redistribution and removal. Our experiments provided insights on the fundamental physics governing the cleaning process, such as the role of the initial conditions and the impact of process parameters on the decontamination efficiency (e.g., needed amount of cleansing resources and washing time).

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References:

Multi-scale Modeling of Dense-Phase CO₂ Decompression for Pipeline and Well Depressurization Applications

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Underground Carbon Storage (UCS) is a powerful technology. CO₂ captured at point sources is transported in its dense phase via pipelines, and injected into suitable deep underground formations. It is important to characterize and quantify the leakage risks associated with this process for its effective design. CO₂ leakage is typically classified into chronic and acute categories (Jordan and Carrey, 2016) based on leakage rates and duration. The latter, also known as blowout events, are Low Probability High Consequence (LPHC) type events.

Well and pipeline blowouts result in the quick decompression of supercritical or liquid CO₂, as it is released into ambient air. This process involves strong Joule-Thomson cooling, often resulting in temperatures below its triple point (−56.6°C). Additionally, the CO₂ outflow through small holes and cracks during the decompression is known to attain sonic speeds (Munkejord *et al.*, 2020). At temperatures below −75°C, one can expect Ductile-to-Brittle Transition (DBT) of steel used in pipelines, exacerbating the leakage. In this work we present a multi-scale, physics-based framework to model Dense Phase Decompression (DPD) during pipeline depressurization, and blowouts of CO₂ injection wells.

For well blowout modeling, we use a 1D CO₂ well flow model coupled with a reservoir simulator. The CO₂ flow within the well is non-isothermal, and accounts for supercritical-liquid-gas-solid phase transitions. For pipeline failure modeling, wherein local temperature effects and leakage hole geometry are important, we employ a 3D flow model. Both, the well blowout and pipeline leakage simulators use a Godunov scheme capable of capturing shocks within sonic flows. The Homogeneous Equilibrium Model (HEM) is employed to simulate complex phase change behavior of CO₂. Additionally, a suitable $k-\epsilon$ turbulence model is employed for the jet flow zone in our 3D pipe failure simulations. Both models account for the conjugate heat transfer between CO₂ and the pipe/well materials during DPD, using Nusselt number correlations for turbulent internal convection.

We present verification studies of our models, compared with published experimental data. We also present sample simulations of i) a two-week-long injection well blowout, and ii) pipeline depressurization. We conclude by discussing future directions and tasks in the project.

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Characterizing Subsurface Hydrogen Migration using Neutron Imaging

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Co-authors: Bijay K C¹; James Torres²; Yuxuan Zhang²; Alexander Long¹; Chelsea Neil¹; Eric Gultinan¹; Hakim Boukhalfa¹; Timothy Germann¹; Michael Gross¹

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Geologic storage of hydrogen (H₂) and natural H₂ exploration are active research areas supporting the energy transition through the use of H₂ as a clean burning fuel. H₂ is expected to see massive demand in the coming decades, which can be facilitated through H₂ generation from excess renewable sources and through accessing natural H₂ reserves. For these operations, it is critical to understand H₂ migration through geologic media. As such, developing an understanding both in traditional porous formations like sandstone rocks as well as ultralow permeability caprocks like shale is important. Here, we develop an experimental capability for studying H₂ migration in cylindrical rock samples using neutron imaging. The application of neutrons works effectively with H₂ unlike X-rays where a secondary contrasting fluid is required. We prepared simplified Aluminum pressure cells and secured the rock samples with epoxy. H₂ was injected from one end while the other end was sealed. Blank neutron images were acquired before the introduction of H₂ and images were collected as the sample was pressurized with H₂. Two pressure values of 50 and 100psi, and three different rocks including Amherst Gray sandstone, Indiana limestone, and a shale sample were tested. Results showed that the movement of H₂ could be successfully captured using neutron radiography. Furthermore, the more porous sandstone and limestone samples showed H₂ intensity which was distinct from the signature for the shale sample. Lastly, the observed changes in H₂ signature were found to be immediate with pressurization and changed minimally over time. This work provides the first application of neutron imaging to study H₂ transport through reservoir rocks and caprock.

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References:

MS06-B / 583

Unstable dynamics of two-phase displacement in porous media associated with hydrogen storage

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Hydrogen storage in saline aquifers offers a promising large-scale, long-term strategy for renewable energy storage. Compared to conventional CO₂ geological storage, hydrogen injection introduces unique challenges due to its ultra-low viscosity and density, high rock reactivity, and microbial driven consumption [1]. In this work, we set aside bio-geo-chemical reactions to focus on the first-order dynamic behavior of the system—hydrogen plume migration during and after injection. Its complexity arises from two potential mechanisms: (1) the large viscosity contrast between hydrogen and brine, which can drive viscous fingering, and (2) the density contrast that may promote gravity segregation. Recent core-scale experiments [2, 3] have shown that these combined effects can induce strong flow channeling and significant hydrogen trapping, highlighting the need to systematically investigate the interplay among capillary, viscous, and gravitational forces across different scales.

To address this gap, we present a three-dimensional dynamic network model for hydrogen–brine displacement, where the solid matrix is represented by realistic rock microstructures, and a two-pressure formulation is employed to resolve corner flow in detail. While this framework was originally built for a strong drainage regime [4, 5], we extend it to incorporate rich pore-scale invasion events that account for different contact angles. We inject a less viscous and less dense fluid vertically into a brine-saturated matrix for a prescribed time, then stop the injection to observe the subsequent fluid migration. We study the displacement patterns at three dimensionless parameters—capillary number, bond number, and viscosity ratio—which are rationalized via linear stability analysis. Furthermore, by comparing our results with core-scale experiments, we reveal the essential physics governing unstable displacements and provide guidance for reservoir-scale simulations of hydrogen storage.

Country:

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MS18 / 584

Impact of water table fluctuations on the redistribution of light hydrocarbons in heterogeneous porous media and remediation efficiency using non-Newtonian fluid flushing

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Contamination of subsurface environments by light petroleum hydrocarbons is a significant environmental issue caused by the widespread use of such products. These hydrocarbons, characterized by their toxicity and low water solubility, pose serious risks to ecosystems and human health. Understanding the transport and fate of these pollutants in the subsurface is crucial for developing effective remediation strategies. Upon release, the pollutants migrate through the subsurface and eventually reach the groundwater table, where significant redistribution occurs due to fluctuations in the water table. Accounting for these fluctuations is critical for effective management of contaminated sites.

This study investigates the redistribution of light petroleum hydrocarbons at the interface between saturated and unsaturated zones under varying water table conditions. Laboratory experiments were conducted to explore the effects of water table fluctuations, soil heterogeneity, and hydrocarbon type on contaminant behavior. The study employed geophysical sensors, image analysis, and remediation testing to characterize these processes.

The experimental setup consisted of a one-dimensional column made of polyvinylidene fluoride (PVDF), measuring 65 cm in height and 10 cm in inner diameter, with a transparent front panel for visual monitoring. The column was equipped with four Time Domain Reflectometers (TDRs) positioned at different heights to measure relative permittivity, and paired pressure ports to simultaneously record pressure data. Relative permittivity values were converted into saturation data using the Complex Refractive Index Model (CRIM) for three-phase fluid flow analysis.

The experiments utilized a heterogeneous porous medium composed of two silica sand grain sizes: fine sand (0.6–0.8 mm) and coarse sand (1–1.25 mm). This setup simulated three subsurface zones: a water-saturated aquifer, a hydrocarbon layer floating above the water table, and an unsaturated soil zone. Diesel oil, representing a typical light hydrocarbon pollutant, was used in the experiments.

The study focused on the effects of imbibition (displacement of non-wetting phases by wetting phases) and drainage cycles, followed by remediation attempts using surfactant and polymer-based flushing agents. Sodium dodecyl sulfate (5 g/L) and xanthan gum bio-polymer (1 g/L) were tested for their effectiveness in displacing the residual hydrocarbons. Experiments included various heterogeneity configurations, such as horizontal and vertical layering, to replicate field-like conditions. Additionally, a complex mixture of degraded hydrocarbons from a pilot site was tested to expand the applicability of the findings.

Preliminary results revealed significant residual diesel saturation in the smear zone, attributed to the hysteresis effects observed during three-phase flow processes. Capillary forces, stronger in smaller pores due to higher entry pressures, played a major role in redistributing hydrocarbons toward zones with higher permeability. This redistribution resulted in lower residual saturation levels in the medium.

Soil heterogeneity was identified as a critical factor affecting hydrocarbon redistribution during imbibition and drainage. These findings underscore the necessity of incorporating heterogeneity into the design of remediation strategies. Additionally, ongoing tests aim to evaluate the behavior of more viscous fluid mixtures and their redistribution pathways, which differ significantly from diesel. Results from these experiments will provide further insights into the dynamics of hydrocarbon behavior and will be presented in the presentation.

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Poster / 585

Interaction between water and point defects inside volume-constrained α -quartz: An ab initio molecular dynamics study at 300 K

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Quartz-based minerals in earth's crust are well-known to contain water-related defects within their volume-constrained lattice, and they are responsible for strength-loss [1-3]. Experimental observations of natural α -quartz indicate that such defects appear as hydroxyl groups attached to Si atoms, called Griggs defect (Si-OH), and molecular water (H₂O) located at the interstitial sites. However, factors contributing to the formation of Griggs and interstitial H₂O defects remain unclear. For example, the role of point defects like vacancy sites (O²⁻ and Si⁴⁺), and substitutional (Al³⁺) and interstitial (Li¹⁺, K¹⁺, Ca²⁺, Mg²⁺, etc.) ions has remained largely unexplored. Here, we performed ab initio molecular dynamics at 300 K to examine the energetics and structure of water-related defects in volume-constrained α -quartz. Several configurations were systematically interrogated by incorporating interstitial H₂O, O²⁻ and Si⁴⁺ vacancies, substitutional Al³⁺, and interstitial Li¹⁺, Ca²⁺ and Mg²⁺ ions within α -quartz. Interstitial H₂O defect was found to be energetically favorable in the presence of Substitutional Al³⁺, and interstitial Ca²⁺, Mg²⁺, and Li¹⁺. In the presence of O²⁻ and Si⁴⁺ vacancies, H₂O showed a strong tendency to dissociate into OH—to form Griggs defect—and a proton; even in the presence of substitutional and interstitial ions. These ions distorted the α -quartz lattice and, in the extreme case, disrupted long-range order to form local amorphous domains; consistent with experimental reports. Our study provides an initial framework for understanding the impact of water within the crystal lattice of an anhydrous silicate mineral such as quartz. We provide not only thermodynamic and process-related information on observed defects, but also provides guidelines for future studies of water's impact on the behavior of silicate minerals. Our findings are published in the Journal of Applied Physics: <https://doi.org/10.1063/5.0190356>.

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586

Comparative Analysis of the Hydraulic Properties of Commercial Gas Diffusion Layers - a Numerical Approach

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The Gas Diffusion Layer (GDL) is a porous part of the fuel cell and electrolyzers that influences the mass transfer in the devices, which has led to a number of studies on its flow properties, including permeability, by different authors. This study conducted single-phase and two-phase flow simulations for four commercially available GDLs utilizing the OpenFOAM computational framework, which employs the finite volume. These simulations allowed for the determination of both the in-plane and through-plane absolute permeability, as well as the relative permeability. Simulations reveal that the permeability of the GDL is influenced by various factors such as porosity, rib compression, fibre size, and pore size distribution. However, the permeability at a given moment in the GDL is determined by a combination of all these properties, including fibre density and alignment. For instance, despite the Sigracet SGL 25 BA having a lower porosity than Toray TGP-H 60 and being more susceptible to rib compression, its permeability values are higher than Toray TGP-H 60. This can be ascribed to additional characteristics such as its greater pore size, larger fibre size, and lower fibre density. Hence affirming the multifaceted interplay of these parameters in determining the overall transport characteristics within the GDL. The results of our findings enable informed decisions when choosing a specific GDL based on our operational goals or the other components within the electrochemical device, such as the type of flow channel or the presence of MPL.

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Deep Learning to predict Oil Volume Production in Pore-Scale Two-Phase Flow

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Deep neural networks have been explored in predicting single-phase flow properties within pore-scale porous media domains. However, their application to two-phase flow scenarios is limited in the literature.

The complexity of two-phase flow arises from fluid-fluid interactions, domain geometry, and the non-linear behavior at the fluid interface. Additionally, porous media domains are not homogeneous, which significantly alter flow outcomes with geometry change.

This study focuses on predicting oil volume production curves in two-phase flow within pore-scale porous media, incorporating the effect of varying fluid viscosities. The deep learning models developed to solve flow cases considering high capillary numbers, indicating dominant viscous forces over capillary forces. The inferred oil volume production curves could be applied to compute porous media properties, such as relative permeability curves.

To train the proposed Machine Learning models, we generate a synthetic porous media dataset using Voronoi diagram patterns, and solve the two-phase flow using the finite element method.

Two neural network architectures are explored: a Convolutional Neural Network (CNN) and a Deep Operator Network (DeepONet). The CNNs are the standard tool used when dealing with image-like data in the Machine Learning context. Moreover, previous works successfully applied CNNs to predict porous media properties, mainly in single-phase flow cases. The DeepONet is a Network structure designed to approximate complex relationships by combining separate inputs into a unified output. Therefore, it takes different non-correlated inputs that interfere on the answer separately and merges the separate functions in the end of the structure. The adoption of DeepONet concept improved the model metrics when compared to the standard CNNs.

Our results indicate that the DeepONet architecture outperforms the CNN, achieving a 45% lower mean squared error in predicting oil volume curves. Additionally, the proposed approach demonstrates robustness by generalizing to different viscosity ratios, enabling predictions of two-phase flow properties across diverse scenarios with varying oil viscosities.

The proposal is shown to be a robust solution to make quick assessment of oil-volume production in porous media, being this inference orders of magnitude quicker than the computation through Finite Element Method solution of the flow.

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MS07 / 589

Non-intrusive global-local method for the poroelasticity model with localized pressure effects

Authors: Hemanta Kunwar¹; Sanghyun Lee²; Son-Young Yi¹

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In many poroelasticity applications, which involve the coupling of mechanics and fluid pressure in porous media, the effects of pressure are often restricted to a limited local region within the entire domain. Thus, solving the poroelasticity system across the entire domain can be computationally inefficient and possibly unnecessary. Alternatively, one can consider solving the full poroelasticity problem only in a local domain where the pressure effect is significant, while solving a simpler linear elasticity problem elsewhere. The resulting model can be seen as an elasticity-poroelasticity interface problem with appropriate transmission conditions.

We propose a non-intrusive global-local algorithm for solving the coupled elasticity-poroelasticity model. In this framework, we iteratively solve the elasticity problem in the entire (global) domain and the poroelasticity problem in the local domain, while ensuring that the transmission conditions across the original interface are satisfied. Although the concept of the global-local algorithm has been previously utilized to address localized nonlinearities in single-physics problems, this study extends the approach to a coupled multi-physics system.

Our approach greatly reduces computational cost, especially when the size of the local domain is much smaller than the global domain. Additionally, the fact that the elasticity problem is solved in the entire domain without compromising accuracy makes this method an attractive alternative to traditional numerical methods, such as domain decomposition methods—particularly when the local domain varies with time or its geometry is complex.

Numerical experiments demonstrate the robustness and accuracy of the proposed method, showcasing its potential for providing scalable and efficient solutions in multi-physics problems where the effect of a single physical process is localized.

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MS01 / 590

Practical Demonstration of Dissolved Gas Injection for Geo-sequestration on Coalbeds

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Conventional geo-sequestration strategies have focused primarily on storage in deep saline aquifers, where DOE low-high estimates of US/Canada potential storage dwarf those of unmineable coal by factors of 40-200x. However, the multifarious challenges of deep aquifer storage have protracted its development and immediate application. Many of these challenges might be addressed by unconventional storage in shallow unmineable coal, including formation integrity and the high cost of capture, purification, compression, pipelines, transportation, and monitoring. Latent geological processes have already amassed hundreds of gigatons of gas in coalbeds as natural gas resource that is well characterized and already exploited by the energy industry. DOE/NETL have stated: 'Coal adsorbs CO₂ over methane...at a ratio of 2 to 13 times. This...adsorption trapping is the basis for CO₂ storage in coal seams.' Nevertheless, early ECBM field trials, which sought to displace natural gas through injection of pure CO₂ to fill the pore space for storage, found insufficient economic benefits from the process. Carbon GeoCapture has revitalized the approach and adapted it to produce a practical, scalable and commercial method for coal geo-sequestration that injects gas in a more natural way. Water sourced from peripheral wells in the coalbed is pumped to surface and mixed with CO₂ gas in a central wellbore to form a dilute dissolved gas fluid that can be readily flowed through the formation. Because the mass fraction of gas in the fluid is low, any potential coal swelling and injectability loss are effectively eliminated.

WellDog has performed laboratory studies that demonstrate and quantify the displacement of sorbed methane on submerged coal through injected carbon dioxide and have developed a benchtop practical demonstration apparatus that illustrates the key steps in the Carbon GeoCapture sequestration process. The system consists of three main compartments driven with a single pump and connected by plastic tubing with automated valving to control mixing and direct flow. During the demonstration, which lasts ~25 minutes, injection fluid is prepared in the first compartment, a vertical Plexiglas column that represents the injection wellbore. Gas is bubbled through the fluid, or fluid from the base of the column is poured into the top of the compartment while equilibrium is monitored with a pressure gauge. The second compartment consists of a series of clear PVC tubes packed loosely with sieved coal cuttings having a void space filled with water pressurized to 50 PSI to simulate formation pressure. During injection, fluid from the first compartment flows through the coal tubes, while displaced fluid is collected in the third compartment, another vertical Plexiglass column that represents the peripheral production wellbore. Displaced fluid from the coal tubes is observed to have significantly less dissolved gas as compared to the injection fluid, which can be dramatically visualized by depressurizing the two vertical compartments simultaneously, where many more bubbles are observed in the injection tank. Even more dramatic is the expansion of gas in the coal tubes when they are depressurized, where sorbed gas expands and displaces all of the water in the pore space.

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References:

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MS25 / 591

Mineralization-Induced Permeability Enhancement for Concurrent Carbon Storage and Critical Mineral Extraction from Ultramafic Intrusions

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To abate the effects of global climate disruption, removal and storage of atmospheric CO₂ will be paramount to decrease the greenhouse effect. Subsurface carbon mineralization in mafic-ultramafic rocks has been demonstrated to permanently store injected CO₂ as carbonate minerals. Ultramafic rocks, have typically higher reactive storage potential compared to their mafic counterparts, yet lack extensive pore and fracture volume for injection. These reservoirs can also have potential applications for geologic hydrogen generation and critical mineral mobilization during carbonation. Thus, increasing reactive surface area is paramount to access the vast reactive potential of these reservoirs. In this study, we performed elevated temperature and pressure reactions with CO₂, meant to mimic geologic conditions, on coarse grain olivine peridotite cubes from the Tamarack Intrusive Complex in northern Minnesota, USA, provided Talon Metals. Samples reacted in both aqueous CO₂ and supercritical CO₂ and with and without organic ligand additives, showed extensive carbonation and fracturing across grain boundaries. The carbonation products were analyzed via micro-X-ray diffraction and SEM-EDS and fracture networks were mapped with X-ray microtomography, showing a significant increase in reactive surface area, with carbonation occurring in fractures.

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MS20 / 593

Modeling the consolidation of a cylindrical poroelastic composite and application to the optic nerve

Authors: Denis Kucherenko¹; Arina Korneva¹

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The mechanical behavior of the optic nerve is largely unknown but is of critical importance to understanding injury and subsequent visual dysfunction from mechanical trauma or elevated intracranial (brain) pressure. The structure of the optic nerve resembles a cylindrical composite with an outer

elastic layer and an inner biofluid-saturated porous core. Current computational and material models do not fully capture the complexities of this tissue's structure, particularly the biofluid has not yet been considered as a load-supporting material.

We developed an analytical model for a cylindrical composite using the theory of poroelasticity. We determined how the solid deformation of the composite is coupled to fluid flow, based on the model of poroelastic soil consolidation by initially developed by Karl von Terzaghi. The expression for the consolidation constant for the composite cylinder was found. We systematically investigated how variations in the geometry and material properties of the outer layer and the inner core of the composite affect the consolidation constant, and therefore the fluid flow, stress, and deformation. The consolidation process of the cylindrical composite depends on the radius of the outer and inner cylinders and their material properties. Sets of parameters can be found where the outer cylinder does not affect the consolidation process of the inner, poroelastic, core. However, these parameters are not appropriate for the optic nerve. Therefore, the outer layer of the optic nerve significantly affects the fluid flow and consolidation behavior of this tissue and has implications for clinical models.

We also modeled uniaxial tension or compression of this cylindrical composite in the absence of fluid draining—when the composite cylinder is sealed. Here, the internal stress is distributed between the layer surrounding the optic nerve, the solid skeleton of the core, and the fluid. Literature values for the magnitude of the compressive or tensile stress were applied to the optic nerve. The results show that the fluid pressure in this tissue can be as large as one third of the applied stress and as high as 120Pa (0.017psi). This magnitude may be significant to injure the nerve. The work stimulates future investigations into the role of fluid pressure during deformation of the optic nerve. The model also provides a framework for experimentally measuring material properties of composite biomaterials subjected to uniaxial tension or compression. We are currently validating the analytical model against creep experiments of pig and cow optic nerves. Our preliminary findings show that the creep behavior can be modeled as consolidation of the composite cylinder, therefore more specimens will be tested.

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References:

596

Optimizing Hydrogen Storage in Alberta's Edson Formation: A Feasibility and Capacity Assessment

Authors: Xiao Yang^{None}; Shengnan Chen^{None}

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Alberta is the largest hydrogen producer in Canada using renewable electricity or natural gas decomposition. Renewable energy sources like solar and wind produce excess electricity during the summer but generate less in the winter. Underground hydrogen storage is seen as a promising solution to store this surplus energy during peak seasons for later use in the winter. This paper aims

to evaluate the feasibility storing hydrogen in a near-depleted gas reservoir in Edson formation, Alberta, as well as the hydrogen storage capacity.

Field data on geology, reservoir fluids, and production are collected for a selected area in Edson formation, where the current recovery factor for natural gas sits at 82%. A comprehensive reservoir model is built and matched towards a production history since 1980s. Multiple hydrogen storage mechanisms are simulated in this study, including structural trapping, diffusivity, solubility, and permeability hysteresis. Different storage scenarios are proposed as storage strategy such as employing historical top producers, existing producers with better reservoir coverage and producers with preferable elevation distributions. In addition, the timing for converting the natural gas reservoir to hydrogen storage is also analysed where the remaining natural gas is employed as the ideal cushion gas. A new multi-objective sparrow search algorithm is further adopted to maximize the H₂ storage capacity and recovery rate through the minimal wells.

Results show that it is feasible to store hydrogen in the depleted gas reservoir. As well injection rate increased, the storage capacity initially increased then stabilized, while the hydrogen recovery rate initially dropped from 47.40% to 34.15%, before increasing again to 39.80%. 7 wells were selected as working wells based on their productivity and location among 29 following wells. Scenario analysis reveals that neither the well highest productivity nor the well located at the top achieved the best recovery rate. Optimization study further confirms that well location, hydrogen injection rate and injection time collectively lead to a highest storage capacity and recovery factor, which is nearly higher 10% than base case. In addition, the difference in hydrogen recovery rate is minimal with and without considering diffusivity and solubility, but cannot be ignored when permeability hysteresis or cushion gas are included.

This research estimates the hydrogen storage feasibility in an actual depleted gas reservoir in Alberta. The findings of this study could potentially pave the way for a more sustainable and efficient energy storage solution. By comparing conventional injection-production schemes, which involve injecting cushion gas and hydrogen into the same wells, with proposed schemes that use different wells for injection and production, a more efficient injection-production strategy is identified. The proposed optimization method provides a feasible approach to prevent local convergence issues and accelerate global convergence, thereby improving the overall effectiveness of the hydrogen storage process.

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Poster / 597

The Implications of Anisotropic Relative Permeability in Commercial Scale Geologic Carbon Sequestration in Heterogeneous Formations

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Geologic carbon sequestration (GCS) as a greenhouse gas mitigation method is reliant on the long-term retention of carbon dioxide within reservoir storage zones. During the subsurface migration of carbon dioxide in highly homogeneous formations, fluids tend to quickly migrate upwards and accumulate at the top of the storage interval. These accumulations are therefore dependent on the surface between the reservoir and the overlying, impermeable zones, i.e. caprocks. This setting leads to capacity being largely dictated by the presence and nature of the structural features of the reservoirs. In the industrial development of GCS, large volumes of CO₂ must be injected to make an impact, and the requirement of structural traps may be limiting or prohibitively costly. On the other hand, highly heterogeneous systems often possess stratigraphic features within the reservoir which impede this vertical migration resulting in higher residual trapping and potentially more laterally compact CO₂ plumes. These formations may be preferential and expand the set of possible storage locations. At the reservoir scale, the stratigraphic heterogeneity that leads to this phenomenon can be characterized through anisotropic relative permeability input curves reservoir models. These models can then be used as predictive tools showing the CO₂ migration dynamics in these heterogeneous formations.

To test this problem, we employed GEOS, a reservoir simulation software package that we expanded to include directional relative permeability hysteresis. We treat relative permeability as a tensor giving us the ability to input different flow properties for different directions. Depending on the level of heterogeneity, different input curves are used for the horizontal and vertical directions aligning with the principal axes of variation. To focus on industrial field development, we created a synthetic, commercial-scale (approximately 14 km by 14 km by 200 m) geologic reservoir model based on a real geologic basin. A series of CO₂ injection flow simulations were executed on this model. The simplest model only includes heterogeneity for porosity and permeability through standard geostatistical well-log derived spatial distribution. Increasingly sophisticated physics models were included to represent heterogeneous and anisotropy using different capillary pressure and relative permeability models. The most complex uses an advanced rock-type model characterization for relative permeability anisotropy and hysteretic anisotropy properties that are representative of the geology's heterogeneity. The results of these simulations and the implications for either ignoring or including these effects are discussed. Results show significant differences in predicted trapping, mobility, and displacement (CO₂ plume footprint). Therefore, when modeling these heterogeneous reservoirs, it may be critical to adopt similar anisotropic models.

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MS05 / 598

Extracting microplastics from water using biofilms grown on pervious concrete

Authors: Adrienne Phillips¹; Kayla Bedey¹; Michael Berry¹

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Microplastics are ubiquitous contaminants where particle sizes are < 5 mm. They are easily mobilized and transported from terrestrial to aquatic environments via storm and surface water runoff

and are consequently found globally in diverse ecosystems. In the effort to reduce microplastic transport, biofilms offer a promising solution. This work presents the first steps in integrating biofilms with concrete flatwork infrastructure, such as sidewalk pavers, by using pervious concrete as the substratum for biofilm growth. Unlike traditional concrete mix designs, pervious concrete omits the use of fine aggregates (i.e., sand) creating pore space within the concrete matrix which allows water to pass directly through it. The high porosity of pervious concrete can support stormwater management and benefit biofilm growth for particle trapping. Methods were developed to grow biofilms on different mix designs of pervious concrete in concrete-filled columns achieving cell densities of 10^7 cfu/g concrete, with the goal of injecting microplastic solutions through the biofilm to assess particle transport and capture. Microplastic solutions were initially passed through columns containing concrete without biofilms to determine any baseline particle capture with the concrete alone using FlowCam analysis to assess the particle concentrations. It is anticipated that biofilm will trap the microplastics above the particle capture by concrete without biofilm and FlowCam analysis on influent and effluent samples will be used to calculate removal efficiencies. Image analysis such as with SEM will be used to visualize plastic trapping in biofilms. These initial experiments indicate that biofilms integrated into pervious concrete infrastructure may offer a strategy to trap and extract microplastics from storm and surface water runoff events.

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Student Awards:

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References:

MS09 / 599

Pore-scale reactive transport modeling for heterogenous in-situ carbon mineralization in partially-saturated vesicular basalts

Author: Tianxiao Shen¹

Co-authors: Olivia Terry ¹; Quin Miller ²; Nabajit Lahiri ²; Shaina Kelly ¹; Todd Schaef ²

¹ *Columbia University*

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A comprehensive understanding of crystallization mechanisms at the pore scale is necessary to accurately predict the kinetics of in-situ carbon mineralization in basalt formations. In this study, we use a finite-volume pore-scale Reactive Transport Model (RTM) augmented by CFD-based CO₂/brine phase distribution and experimentally-informed geochemistry kinetics to understand the dynamic precipitation process of various carbonate phases at the Wallula Basalt Injection Project, where 1000 MT of dry supercritical CO₂ was injected over a 25-day period followed by a 2-year shut-in period. Petrographic data (e.g., optical microscopy, SEM, micro-CT) from post-injection sidewall cores collected from three permeable flow-top regions indicate that in-situ carbon mineralization primarily proceeds through heterogeneous nucleation inside geometrically-isolated vesicles, resulting in a variety of chemical-zoned carbonate nodules with different geometries and surface-area-to-volume ratio. However, as the detailed pore-scale processes are not yet well understood, the time series of these processes remain insufficiently constrained by the bulk site monitoring data (e.g., well logs,

produced water chemistry) from the Wallula site, hindering reliable predictions for in-situ mineralization inside basaltic formations.

Specifically, we focus on recreating a diffusive- and surface-tension-dominated transport regime inside isolated vesicle systems in the flow top zones over a 2-year post-injection period. Informed by further pore-size analysis (e.g., NMR and BET) and elemental & crystallographic analysis (e.g., EDX, XRF, XRD, TEM), our preliminary analysis of pore-scale carbonate chemistry and morphologies revealed that: 1) inter-vesicle advection of CO₂ and diffusion of major cations (Fe²⁺, Mn²⁺, and Ca²⁺) is negligible over the 2-year post-injection period, and 2) pore-lining clays serve as the primary cation source during the early stages of post-injection geochemical processes. Therefore, these isolated vesicles were treated as natural batch reactors in the pore-scale RTM simulation with closed boundaries and a self-sufficient cation source during the post-injection period.

Starting from the two-phase brine/sc-CO₂ distribution caused by initial pressure-driven flushing during injection, we explored how dissolution and diffusion of carbonate species control pH and supersaturation distributions within partially saturated vesicles. Lab-scale titration experiments informed the mass transfer rates of cations from pore-lining clays, driven by local Eh-pH conditions. Using a transition-state-theory-based equation, we modeled carbonate growth dynamics to predict the final 3D morphologies of carbonate nodules. Dynamic properties include carbonate surface-area-to-volume ratios, brine/CO₂ and brine/mineral interfacial area, and local pH distribution as a function of saturation state, precipitation rate (Da#), and time-lapse inside isolated basalt vesicles.

Our reconstructions of these dynamic geochemical processes were compared with produced water chemistry from the Wallula site to validate our predictions. Going forward, we are looking into how these pore-scale dynamic processes may be upscaled into gridblock-based reservoir simulators (e.g., STOMP-CO₂, PFLOTRAN) through continuum-scale variables such as pH and water saturation. We posit that this proposed simulation workflow provides a comprehensive understanding of pore-scale processes that complements current observations and supports more reliable predictions of in-situ carbon mineralization.

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References:

MS15 / 600

Nowcasting and forecasting soil moisture using meteorological parameters

Authors: Hassan Dashtian¹; Michael Young¹

¹ *University of Texas at Austin*

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Real-time, high-resolution estimates and predictions of soil moisture (SM) data could significantly enhance the forecasting of SM- and precipitation-related extreme events, such as floods, droughts, and wildfires. Current estimates and short-term predictions of SM data can serve as leading indicators for upcoming anomalies in vegetative growth and productivity, improve irrigation scheduling, and enhance streamflow forecasting. However, existing SM data products—including in-situ measurements, satellite-derived data, and model-derived simulated reanalysis data—are valuable but fall

short of simultaneously providing real-time, high-resolution, broad spatial coverage, and near-future estimates of soil moisture.

In this study, we propose a deep learning (DL) framework that integrates historical satellite-derived SM data, in-situ measurements, and meteorological data to address these limitations. The framework is designed to reduce the latency between satellite-derived SM data release and the current time, thereby offering more up-to-date SM estimates. Furthermore, we forecast SM for the next 11 days using meteorological inputs such as precipitation, air temperature, humidity, wind speed and direction, and solar radiation.

Our framework aims to deliver more timely SM estimates by minimizing data latency while also providing short-term forecasts of SM. The primary objective is to generate real-time, high-resolution SM estimates for the entire state of Texas. Currently, real-time, up-to-date SM data and predictions are not available at this resolution or scale. To address this gap, we employ meteorological data to guide a DL model that estimates and predicts NASA's SMAP Level 4 SM data product, which currently has a latency of 2–5 days.

Our DL model is specifically designed to account for both the temporal and spatial heterogeneity of SM. It is deployed in an “on-line” fashion, meaning the model is trained continuously as new data becomes available. This iterative updating process allows the model to adapt dynamically to changing patterns over time, ensuring that predictions remain accurate and relevant in real-time.

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MS03 / 605

Effect of Pressure and CO₂ Solubility on Etch Pit Formation in Fractured Peridotite

Author: Hoang Nguyen¹

Co-authors: Wenfeng Li ¹; Luke Frash ; Hari Viswanathan ¹; Chelsea Neil ¹; Uwaila Iyare ¹

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To achieve the goal of limiting the global temperature increase to below 2°C and avoid the adverse effects of climate change, the removal of CO₂ from the atmosphere requires the simultaneous application of carbon capture, utilization, and storage (CCUS) methods. Among these, carbon mineralization is a promising approach that can securely trap a substantial amount of CO₂. Ultramafic rocks, such as peridotites, are rich in minerals like olivine and pyroxene, which can react with CO₂ to form solid calcite and magnesite through dual dissolution-precipitation processes. However, these ultramafic rocks are notoriously low in permeability, and mechanical cracks have been proposed to increase the reactive surface area [1]. A previous study [2] suggested that dissolution and precipitation were spatially decoupled in the presence of advective or convective flow through the cracked solid. Multiple etch pits resulting from the dissolution process were observed on the surfaces of the reacted olivine grains and could facilitate further cracking. However, the formation mechanisms of these etch pits, including their size, shape, and density under realistic conditions such as shear cracks subjected to high confining pressures and fluid with variable CO₂ contents and flow rates,

remain unclear. To address these uncertainties, we conducted a core-flooding experiment using both aqueous and wet super critical CO₂. The aqueous CO₂ was premixed at various temperatures and pressures to generate different CO₂ solubility levels. Using a triaxial direct-shear (TDS) system, we induced shear fractures in the peridotite core under subsurface temperature and pressure conditions. These fractures exhibit small-scale geometrical characteristics, such as tortuosity, roughness, aperture distribution, and asperity contacts, that are representative of subsurface cracks and critical for etch pit formation, crack evolution, and reaction transport. Following the creation of the shear cracks, we evaluated the absolute permeability of the fractured core under different effective confining pressures. Effluent samples were collected for each permeability measurement and analyzed using inductively coupled plasma–optical emission spectroscopy (ICP-OES) to monitor elemental changes, providing insights into mineral dissolution. High-resolution X-ray computed tomography (~45 µm) was used to visualize etch pit formation and the subsequent evolution of crack networks. Post-experiment analysis of the fractured surfaces using scanning electron microscopy (SEM) coupled with energy-dispersive spectroscopy (EDS) unveiled changes in chemical composition within and around the etch pits. The experimental findings provide critical insights for achieving adaptive controls of reactive surfaces, paving the way for sustainable and scalable CO₂ mineralization in subsurface mafic and ultramafic formations.

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MS08 / 608

Residence-timers approach to identify subdomain residence times in composite media like river corridors.

Author: Timothy Ginn¹

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River corridor beds are often comprised of distinguishable subdomains such as the benthic biolayer and the underlying hyporheic zone. Mixing between streamwater and groundwater, that controls reaction extent for a variety of biogeochemical transformations, can occur at dramatically different rates in the different domains including the stream, the benthic layer, the hyporheic zone, or any combination thereof, depending on the characteristics of the river corridor. For instance the time spent in the benthic biolayer by solutes that start in the stream appears to be an excellent proxy for extent of redox reactions controlling transformation of such solutes. Similarly, precipitation/dissolution reactions may occur predominantly in the lower hyporheic sediment layer(s). Thus it would be useful to have a practical means to determine the residence-time distributions of solutes in any of the subdomains (or a combination) for a given river corridor given their starting place. Such a method could be used in gaining an understanding of the extent of transformation of riverine and/or groundwater solutes, given basic properties of the river corridor such as layer thicknesses, porosities, and diffusion coefficients. To develop such a method we expand upon a notion that the steady-state solution to a multi-domain transient mass balance equation system, that has been fitted with ‘residence-timers’ (mathematical clocks) for each subdomain, can give the residence time distribution in the separate subdomains or combinations thereof. We present an overview of how

this works and demonstrate the results for an example system. The solutions obtained are closed-form in Laplace space, and numerical computation only enters in the final step of inverting the expressions obtained to convert from Laplace space to residence time.

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References:

Poster / 609

Experimental Investigation of Fiber-Foam Multiphase Flow

Author: Anthony McMaster¹

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In a 2014 report, the DOE recognized the paper industry as the third largest consumer of energy in the United States, accounting for 13% of the manufacturing energy consumption used nationally. Because water is predominantly the carrier fluid during paper manufacture, evaporative drying at the end of the manufacturing process can account for 2/3 of paper making energy consumption. Accordingly, fiber foams, where the carrier fluid is a bubbly foam, present a path for a predicted 10%-40% energy savings, without sacrificing product quality. To design industrial processing equipment, a representative fiber foam made of aqueous sodium dodecyl sulfate is examined as a function of gas fractions (20% to 80%) and fiber content (0% to 2%). A pressure driven pipe flow apparatus is designed and used to simulate the paper making process. Constitutive models for fiber-laden foam will subsequently inform computational models for designing nozzles and processes that will demonstrate the utility of this carrier fluid for the paper making industry.

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References:**Poster / 610**

Competitive Adsorption of Methane and Carbon Dioxide on High-Specific-Surface Geomaterials: Insights from NMR Relaxation and GCMC Simulations

Author: Camilo Guerrero¹

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¹ *Geosyntec Consultants*

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Abstract. Shales are abundant source rocks for natural gas in sedimentary basins, and gas recovery from shales has gained increased attention given the global rise in energy demand. Despite advancements in horizontal drilling, hydraulic fracturing, and depressurization to atmospheric conditions, recovery rates for natural gas from shales remain limited to 20-60%. This is primarily due to the strong adsorption of methane CH₄ on shale surfaces, highlighting the need for additional stimulation techniques. Enhanced CH₄ recovery via carbon dioxide CO₂ injection into shales is an appealing method due to the ability of CO₂ to displace adsorbed CH₄, facilitating its desorption. Experiments under high-pressure and high-temperature conditions have shown that shales adsorb more CO₂ isothermally than CH₄. Moreover, CO₂ adsorption presents the dual benefit of enabling gas recovery while contributing to CO₂ emission mitigation. This study employs low-field Nuclear Magnetic Resonance NMR measurements to investigate competitive CO₂-CH₄ adsorption in high-specific-surface-area shales, supplemented by sodium bentonite, illite-smectite and kaolinite to simulate key shale components. Low-field NMR offers a distinct advantage over gravimetric and volumetric methods by differentiating between relaxations of adsorbed and free gas phases. Furthermore, in CH₄-CO₂ mixtures, only CH₄ molecules are detectable via ¹H NMR, which enables precise analysis of CH₄ desorption following CO₂ injection. The research is conducted in two stages. First, we analyze the NMR relaxation and adsorption effects of single-phase CH₄ on geomaterials at high pressure and high temperature. Second, we study the time-dependent CO₂-CH₄ competitive adsorption through NMR spectral changes in selected geomaterials. These experiments are complemented by Grand Canonical Monte Carlo GCMC simulations of adsorption on clay mineral surfaces resembling the tested geomaterials, incorporating single-phase CH₄, CO₂-CH₄ mixtures, and He-CH₄ mixtures to analyze competitive adsorption dynamics. Results reveal that the transverse T₂ relaxation response of CH₄ gas in geomaterials exhibits two relaxation peaks at low pressure (P<~1 MPa) and three relaxation peaks at higher pressures (P=2-to-10 MPa), reflecting Langmuir adsorption and the behavior of bulk CH₄ within pores and external to grains. CH₄ desorption triggered by CO₂ injection is governed by two mechanisms: (1) partial pressure reduction of CH₄, a universal response to gas injection, and (2) preferential adsorption of CO₂ on clay minerals due to higher CO₂ selectivity. A modified kinematic desorption equation is proposed to account for the residual adsorbed CH₄ fraction following CO₂ injection. The combined insights from low-field NMR measurements and molecular simulations provide a detailed understanding of competitive gas adsorption at the pore scale, advancing the knowledge needed to optimize enhanced CH₄ recovery techniques.

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MS08 / 611

Diffusiophoretic transport of colloids in porous media**Author:** Mobin Alipour¹**Co-authors:** Haoyu Liu ¹; Yiran Li ¹; Amir Pahlavan ¹¹ *Yale University***Corresponding Author:** amir.pahlavan@yale.edu

Gaining control over the motion of colloids in complex environments is essential in a wide range of applications, from cell sorting and drug delivery to filtration and water purification. Recent studies have demonstrated the utility of diffusiophoresis, ie, the motion of colloids due to solute gradients, in manipulating and steering colloids in simple microfluidic geometries. Yet, it remains a question whether diffusiophoresis could play an important role in more complex environments, with spatiotemporal gradients in solute gradients and flows. Here, combining experimental observations and numerical simulations of microfluidic channels patterned with obstacles, we study the competition between phoretic and convective migration of colloids and discuss its implications on the transport, dispersion, and steering of colloids on macroscopic length scales.

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Poster / 612

Bacterial chemotaxis and dispersion in crowded environments**Authors:** Akash Ganesh¹; Mobin Alipour¹**Co-author:** Amir Pahlavan ¹¹ *Yale University***Corresponding Author:** amir.pahlavan@yale.edu

Swimming bacteria can adapt their swimming in the face of environmental cues and stresses. In response to nutrient gradients, bacteria lower their tumbling frequency when going up the gradients, leading to a net drift toward the nutrient source. In the presence of flows and in crowded environments, however, bacterial swimming patterns change. They get trapped near surfaces due to flow shear, and around obstacles due to hydrodynamic/steric interactions. While bacteria often live in such complex environments, our understanding of bacterial chemotaxis has mostly remained limited to simple environments with 1D steady nutrient gradients. Here, using microfluidic experiments and

numerical simulations, we probe the role of chemotaxis in dynamic environments in the presence of flows and obstacles on bacterial colonization of nutrient sources. We discuss the implications of our observations for bacterial colonization of marine snow in the oceans and nutrient hotspots in the soil.

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MS25 / 613

Investigation of Pore Characteristics for CO₂ Mineralization Through Digital Rock Physics

Author: Hyunjeong Jeon¹

Co-authors: Weon Shik Han ¹; Hyungchul Shin ¹; Chaewon Park ¹; Peter Kang ²; Rhokyun Kwak ³; Kue-Young Kim ⁴

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³ *Hanyang University*

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Despite extensive global efforts to mitigate climate change, CO₂ emissions continue to rise, emphasizing the necessity of geologic carbon sequestration (GCS). CO₂ mineralization is one of the effective methods of GCS, using CO₂-fluid-rock reaction; after injection of CO₂-charged water, CO₂ is rapidly and permanently immobilized through carbon mineralization. In general, mafic/ultramafic rocks (e.g., basalt and peridotite) are targeted for CO₂ mineralization due to their huge CO₂ storage capacities with prevalence in the earth's surface and high content of divalent metal cations. For instance, the CarbFix project targeting basaltic rocks in Iceland was successfully conducted in pilot-scale, showing that 95 % of injected CO₂ was rapidly mineralized within 2 years.

It has been found that petrophysical properties such as porosity, permeability and surface area, which depend on pore space that enables fluid flow and reactions, significantly affect CO₂ mineralization and control the CO₂ storage potential of reservoir. Consequently, identifying pore characteristics is crucial for evaluating the impact of rock properties on CO₂ mineralization. Digital Rock Physics (DRP), an advanced technology utilizing micro-CT imaging, allows for the non-destructive assessment of complex pore characteristics in rocks.

In this study, to evaluate the pore characteristics and the effect of the petrophysical properties of mafic/ultramafic rocks on CO₂ mineralization, the DRP workflow, including micro-CT image analysis, was applied to rock samples (i.e., 5 basalt rocks from the CarbFix and Jeju Island in the Republic of Korea, and 1 peridotite). To do, those samples were scanned using the synchrotron at Pohang Light Source, and then high-resolution images with voxel resolution of 1.625 μm were acquired. Then, 3D pore structures of each rock sample were obtained through image reconstruction and segmentation processes, followed by estimation of the parameters such as absolute and effective porosity as well as specific surface area (SSA). Finally, permeability and pore characteristics were quantified by extracting the pore-network model.

The results so far show significant variation in the pore structures, even within the same rock type, resulting in differences in the petrophysical properties. The CarbFix basalts exhibit high porosity (~0.28) and permeability (~10⁻¹³ m²) due to macro-pores, along with high SSA attributed to the distinctive round structure of mineral precipitation. One of the Jeju basalts primarily consists of micro-pores, leading to low porosity (~0.10), but its permeability (~10⁻¹⁵ m²) and SSA are high due to a well-connected pore network and the pore size distribution. The porosity of peridotite is relatively low (~0.03), but its permeability is comparable to that of CarbFix basalt due to the presence of a fracture network. Ongoing research involves numerical modeling to quantitatively evaluate the effects of the petrophysical properties resulting from the pore characteristics on CO₂ mineralization.

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MS25 / 614

Complex Carbonate Phases Drive Subsurface Carbon Mineralization Processes

Author: Nabajit Lahiri¹

Co-authors: Quin R. S. Miller¹; Libor Kovarik¹; Emily Nienhuis-Marcial¹; H. Todd Schaefer¹

¹ *Pacific Northwest National Laboratory*

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In situ carbon mineralization in basalt, is a necessary, yet underdeveloped strategy to mitigate the worsening impacts of climate change. In this regard, the Wallula Basalt Carbon Storage pilot project, led by PNNL, is the world's only field-scale injection of supercritical CO₂ in basalt formations and the only demonstration where rock samples containing anthropogenic carbonates have been retrieved. This presentation highlights our work using atomic-scale microscopy to discover four key mineralization endpoints correlating to the initial and later stages of nucleation and growth of carbonate nodules formed within basalt pores as a result of CO₂ injection. Surprisingly, we discovered that the initial stage of carbonation was controlled by a never-before-seen carbonate phase, a cation-ordered Mg-absent ankerite, despite the near-ambient temperatures. Additionally, we will highlight the critical role played by secondary pore lining phases, such as zeolites, and clay-rich linings, on the nucleation of these elusive carbonates. Overall, the study enables a much-improved geochemical understanding of complex subsurface carbonate formation processes that drive geologic carbon storage in reactive reservoirs. The nanoscale observations in this study provides critical baseline information required for the parameterization of predictive models at the field scale for any future permitting, monitoring, storage validation in basalt reservoirs worldwide.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

MS03 / 615

Evolution of Hydraulic and Mechanical Apertures in Heterogeneous Fractures Driven by Mineral Precipitation

Authors: Ruoyu Chen^{None}; Russ Detwiler^{None}; Mohammad Javad Abdolhosseini Qomi^{None}

Corresponding Authors: detwiler@uci.edu, mjaq@uci.edu, ruoyu.chen@uci.edu

Chemical reactions induced by fluids that are out of chemical equilibrium with the minerals on fracture surfaces lead to mineral dissolution and/or precipitation along fracture surfaces and alterations in the fracture aperture. Incorporating the influence of localized chemical alterations into continuum models requires effective constitutive models that relate changes in mechanical aperture to changes in hydraulic aperture and reactive surface area, which control the concentration distribution within the fracture. Local reaction rates depend on ion concentrations, reaction kinetics, and available reactive surface area. The local ion concentrations are strongly influenced by the relative rates of advective transport of ions through the fracture and local reaction rates, which are characterized by the dimensionless Damköhler number ($Da = kLW/Q$, where Da is the Damköhler number, k is the reaction rate coefficient, L and W are the fracture length and width, and Q is the flow rate). In this study we explore how Da , aperture variability, and mineral heterogeneity influence the evolution of reactive surface area, the mechanical and hydraulic aperture. Our analysis is based on 480 high-resolution mechanistic simulations using a previously developed model that simulates advective-reactive transport within variable aperture and explicitly represents the resulting three-dimensional growth of minerals on the fracture surfaces (Jones and Detwiler, 2019). We varied Da , relevant geometric parameters including fracture aperture (mean, standard deviation, and correlation length) and initial reactive surface area (magnitude and spatial distribution) over the full range of expected parameter values. Our results demonstrate a strong dependence of fracture-scale hydraulic aperture evolution on Da , particularly with the spatial distribution. At high Da , precipitation occurs more rapidly at reaction sites near the fracture inlet than those near the outlet, leading to hydraulic aperture decreasing faster than mechanical aperture. At low Da , reaction rates are more uniform across all reaction sites, and the mechanical and hydraulic apertures evolve at similar rates. Additionally, because reaction rates are uniform throughout the fracture, the evolution of aperture and reactive surface area depends on the geometry of the evolving surface, rather than the distance along the fracture. We propose a constitutive model that relates precipitated volume to reactive surface area. This model enables the development of a simplified one-dimensional continuum framework, effectively representing the influence of mineral precipitation on fracture transport properties over the broad range of parameter space considered in our simulations.

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Jones, T. A. and Detwiler, R. L. (2019). Mineral precipitation in fractures: Using the level-set method to quantify the role of mineral heterogeneity on transport properties. *Water Resources Research*, 55(5):4186–4206.

616

Microfluidic chip evaluation of surfactant effectiveness on enhanced oil recovery: comparing displacement performance in parallel porous structure with similar porosity and different permeability

Author: Vitaly Kazaku^{None}

Co-authors: Alexandra Scerbacova¹; Alexey Cheremisin; Dmitrii Pereponov²; Evgeny Shilov³; Michael Tarkhov⁴

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Objectives/Scope:

In the modern world, the era of easily recoverable hydrocarbons is coming to an end, so the oil and gas industry is increasingly resorting to methods of enhanced oil recovery (EOR), including injection of chemicals (surfactant, polymers, etc.). Traditional screening methods are usually time-consuming and complex, so this paper demonstrates the use of microfluidics as a rapid screening method of surfactants for particular conditions.

Methods, Procedures, Process:

Two selected surfactant compositions based on alkyl ether carboxylates (AECs) with various molecular structures were tested for thermostability at 70°C and 10 different salinities (0% to 20% TDS). Interfacial tension (IFT) measurements were performed at 70°C using a spinning drop tensiometer. A phase behavior test with oil was conducted to evaluate the emulsification ability of AEC-based surfactants in the presence of Na⁺, Ca²⁺, and Mg²⁺ ions. Then, microfluidic experiments were conducted. Microchip structures had same porosity but different permeability of 1x mD, 5x mD, and 10x mD values. The inner surface of microfluidic chips was hydrophobized with a silanization solution.

Results, Observations, Conclusions:

The stability test showed that one surfactant was stable under considered conditions, and it was used in all further experiments. Three samples were selected for microfluidic tests based on their interfacial tension (IFT) values. The increased brine salinity resulted in a 10-fold decrease of the IFT value, reaching 10⁻² mN/m order of magnitude. Phase behavior test in a bulk showed no emulsion or microemulsion formation, but at a salinity of ~20 wt/%, the transition of hydrocarbons into an aqueous phase was observed. Microfluidic studies showed that the structures with higher permeability (10x mD) doesn't exhibited a greater oil displacement efficiency, because of fingering effect. In the structure possessing a permeability of 1x mD, a slow and narrow displacement of oil with a filamentary nature was observed. Conversely, filtration occurred rapidly in the network characterized by 5x mD, and the displacement front was uniformly distributed across the entire width of the structure.

Novel/Additive Information:

This paper presents novel information on using microfluidic chips with close porosity but different permeability for surfactant screening in EOR applications. This study allowed us to visually assess the patterns of fluid behavior within the pore structure and establish a correlation between channel widths and the quantity of oil displaced. The real-time observation of surfactant behavior at the oil-water interface also provides valuable insights into the phase interactions.

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Poster / 617

Exploratory Modeling of the transport of nptII antibiotic-resistance gene and its interactions with ambient DNA in real soil columns

Author: Timothy Ginn¹

Co-authors: Sandra Un Jan Contreras ; Courtney Gardner ; Rajitha Senavirathna ; Rishi Parashar ; Sabrina Volponi

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Use of antibiotic-resistance genes (ARGs) in agriculture is growing as is the recognition of the associated potentially catastrophic threats to human health if such ARGs transfer into pathogenic soil bacteria. Here we summarize previously reported data from our column experiments involving the fate and transport of the ARG nptII in soil from a farm in north-central Oregon, and then detail our approach to simulation of these data. NptII is widely used as a selection marker in genetically-modified crops and is also naturally produced by ambient soil biota. The experiments are designed to evaluate the persistence and motility of nptII in true soils under rain events with contribution of decaying litter to ARG in influent solution. As a result, while the dataset affords observation of transport and interactions in a realistic setting, it has a number of unknowns that precludes predictive modeling. By application of Occam's razor and the casting of several testable assumptions, we developed a modeling approach that works pretty well and more importantly prioritizes new hypotheses for examination. Specifically, we combined an irreversible first-order leaching model for native DNA and nptII, with reversible immobilization for both leached and injected solutes represented via first-order kinetics with memory (Ginn et al., 2017). Further, the data reveal dramatic interaction between injected nptII and native DNA in the effluent samples, for which we develop several simple models for testing. These exercises help in the design of the next suite of experiments.

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Water & Porous Media Focused Abstracts:

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Ginn, T. R., L. G. Schreyer, K. Zamani, Phase exposure-dependent exchange, *Water Resources Research* 53 (1), 619-632; Tiedje, J. M., et al., Antibiotic resistance genes in food production systems support One Health opinions, *Current Opinion in Environmental Science & Health*, Volume 34, 2023, 100492, <https://doi.org/10.1016/j.coesh.2023.100492>.

MS23 / 618

Hydrogen Adsorption in Nanoporous Geomaterials Using Low-Field NMR and GCMC Simulations –Implications for Storage

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Abstract. The conventional gravimetric and volumetric methods used for gas adsorption analyses are unable to differentiate between adsorbed and free gas behaviors and often rely on estimated adsorbed gas densities from molecular simulations for high-pressure corrections. This study introduces a novel approach using low-field Nuclear Magnetic Resonance NMR to gain deeper insights into high-pressure hydrogen H₂ gas adsorption in geomaterials. Our focus lies on gas pressures relevant to near-surface and geological storage applications, which typically range across several MPa. This study employs NMR measurements to investigate the H₂ adsorption capacity and the average density of the adsorbed H₂ monolayer in high-specific-surface-area shales. The analysis is extended to sodium bentonite, illite-smectite, kaolinite, and activated carbon to represent key shale components. Complementary adsorption simulations using Grand Canonical Monte Carlo GCMC on analogous mineral surfaces were employed. Unlike other 1H-containing gases, results reveal two distinct relaxation mechanisms of H₂ gas in porous media: a time-invariable short relaxation indicative of H₂ monolayer adsorption, and a pressure-dependent long relaxation attributed to free H₂ gas in pores. The absolute H₂ adsorption capacity increases progressively from reactive shales to high-specific-surface-area clays and activated carbon. Notably, H₂ storability improves significantly in bentonite at high pressures and in activated carbon across all pressures. Moreover, NMR-derived densities of adsorbed H₂ show values 2.5 to 4 times greater than those of bulk H₂. In addition to the mineral specific surface area, this study highlights the influence of adsorbate molecular packings, molecular orientation distributions within the adsorbed layer, and mineral surface homogeneity on H₂ gas adsorption. Our laboratory results have potential applications for interpreting downhole NMR characterization tools in field studies.

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Dynamics of fluid-driven fractures across macroscopic material heterogeneities

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Fracture propagation is highly sensitive to the conditions at the crack tip. In heterogeneous materials, microscale obstacles can cause propagation instabilities. Macroscopic heterogeneities modify the stress field over scales larger than the tip region. We present an experimental study that investigates the propagation of fluid-driven fractures through multilayered materials. We focus on analyzing fracture profiles formed upon injection of a low-viscosity fluid into a two-layer hydrogel block. The fracture propagates in the toughness-regime. Experimental observations highlight the influence of the originating layer on fracture dynamics. Fractures initiated within the stiffer layer experience rapid fluid transfer into the softer layer when reaching the interface between the two materials. We characterize the propagation dynamics and show that they are controlled by the toughness contrast between neighboring layers. Indeed, the toughness contrast drives fluid flow. We model the coupling between elastic deformation, material toughness, and volume conservation. After a short transient regime, scaling arguments capture the dependence of the fracture geometry on material properties, injection parameters, and time. These results show that stiffness contrast can modify fracture propagation over large length scales and demonstrate the importance of macroscopic scale heterogeneities on fracture dynamics.

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MS04 / 620

Powder X-Ray Diffraction data for swelling pressure interpretation

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In the scope of nuclear waste disposal facilities active clays are beneficial in comparison to other materials due to their higher swelling and sealing abilities. A unique correlation has previously been established between the final swelling pressure and the dry density of MX-80 bentonite. Additionally, it has been demonstrated that the final swelling pressure is independent of the material's fabric. However, validating these findings regarding swelling pressures in the presence of saline solutions remains a significant challenge. Saline solutions are known to induce chemical consolidation in bentonites, reducing the attractive forces within the diffuse double layer (DDL) and increasing

shear strength. This process potentially impacts the final swelling pressure of bentonites. However, the existing data are insufficient to establish a consistent relationship across various fabric types at the same salinity level. Furthermore, the extensive variability in bentonites and their mixtures complicates the aggregation of data across different materials. As a consequence, this study proposes a methodology to utilize available swelling data from different types of sodium-bentonite at varying sodium chloride concentrations to derive a unified swelling pressure-dry density curve. This methodology includes (i) use of the montmorillonite dry density rather than the conventional dry density of bentonite, and (ii) integration of experimental results from Powder X-ray Diffraction (PXRD) to assess the influence of saline solutions on montmorillonite spacing. Using PXRD data, this methodology initially was able to predict the liquid limit across a broad spectrum of saline solutions and to identify a mechanical equivalent of chemical loading. By incorporating the latter, the swelling pressure curve for distilled water was reconstructed from each curve corresponding to a specific salinity level. This approach has been demonstrated to be effective for dry densities above 1.2 Mg/m^3 , enabling the derivation of a unified swelling pressure versus dry density curve for MX-80 and Gaomiaozi bentonites. For lower compactions, a coefficient that accounts for scaling from the nano- to macroscale effects of salinity has been proposed.

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MS06-A / 621

Two-phase flow in porous media under the influence of external electric and magnetic field - Multiscale homogenization approach

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This work provides the derivation of a new model for immiscible flow of a wetting phase inside a non-wetting phase through the pores of a homogeneous porous medium under the effect of external electric and magnetic fields. The model assumes both fluid phases to be incompressible and Newtonian, with the solid matrix being rigid and impermeable. The porous medium, characterized by a length ℓ , is divided into periodically structured regions of smaller length ℓ . For mathematical and physical understanding of two-phase flow, diffuse interface model is used. The interface between the two fluids is governed by the Cahn-Hilliard equation and the influence of electromagnetic fields is incorporated in the Stokes equation by the Lorentz force term. The research employs a two-scale asymptotic homogenization approach to upscale Stokes-Cahn-Hilliard (SCH) equation system and derive the electromagneto(EM)-permeability tensor by extending Darcy's law to account for multiple phases and incorporating the influence of external electromagnetic fields. The finite element method is utilized to solve the derived equations. The results indicate that capillary number (Ca), wetting phase saturation (ϕ_w), the intensities of external magnetic field

defined by the Hartmann number (Ha) and magnitude of external electric field represented by a non-dimensional parameter (S) affect the EM-permeability.

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MS01 / 622

An Integral Model of Gas Diffusion, Sorption, and CO₂ sequestration in Tight Dual-Porosity Organic-Rich Systems

Authors: Ye Lyu¹; Kristian Jessen²

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To optimize shale gas recovery during production operations and subsequent CO₂ storage in depleted shale plays, it is essential to accurately represent all transport and storage mechanisms involved. These include viscous flow, transitional flow, Knudsen diffusion, surface diffusion, and sorption. Despite extensive efforts in technical literature, comprehensive modeling of transport and sorption in fractured shale remains a major challenge.

In our previous research, we introduced a multi-porosity model based on the assumption that the characteristic time for sorption is greatly larger than the characteristic time for transport. Building on that foundation, this study introduces a general dual-porosity model for cores-scale interpretation of gas transport and sorption in organic-rich shales. The new formulation was developed to accommodate gases exhibiting a broad range of sorption affinities and extends the applicability of Vermeulen's generalized modeling approach to a broad range of characteristic times for sorption.

To validate the proposed model, we compare calculation results with fully discretized numerical solutions for inert gases (helium - He) and highly adsorbing gases (i.e., carbon dioxide -CO₂). The comparison demonstrates that the new model provides for accurate representation of gas transport and sorption in dual-porosity systems without the need for full domain discretization. Furthermore, we demonstrate how the new model can be applied to characterize transport and storage in shale cores based on tandem experiments with He and CO₂.

In summary, a novel integral model for transport and sorption in dual-porosity systems is developed and validated. The model is demonstrated to provide an efficient tool for interpretation of core-scale experiments while also offering a path for upscaling transport and sorption via translation of relevant characteristic times.

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625

Microstructural Evolution and Phase Behavior of n-Alkane in an Irregular Nanopore of Shale Formation

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Shale rocks are abundant in nanopores that range in size from 1 to 20 nanometers. Within these small pores, the pore surfaces can significantly influence all fluid molecules within the confined space. This strong pore-fluid interaction and its competition with fluid-fluid interactions could lead to a heterogeneous distribution of fluid molecules in the pore spaces, which results in modified phase behavior. A fundamental example is the capillary condensation phenomenon occurring in a slit-like nanopore (Fig.1a), which has been studied by numerous studies. Figure.1 Illustration of the (a) slit-like nanopore and the (b) semi-closed nanopore model. The pore diameters are d and that could shrink to d' , the adsorbing layers are of the width H , the depth of semi-closed nanopore is w . As we know, capillary condensation in a planar slit can be explained as a simple finite-size shift of the bulk liquid-gas phase transition, controlled by a geometric parameter d (the width of the slit). The basic mechanism of capillary condensation in slits of different pore sizes is the same, but the degree of geometric constraints caused by changes in pore size leads to quantitative differences in capillary condensation behavior at different pore sizes. Specifically, as the pore size shrinks from d to d' , the confinement effect of the pore wall on the fluid strengthens, confined fluid is more likely to condensation at same pressure and temperatures (Fig.1a). On the mean-field level, the gas-liquid phase transition can be determined by constructing adsorption isotherms, calculating the capillary condensation pressure and other parameters of the fluid under different conditions. However, the pore structure in shale formation could be more complex and irregular. It means that the translation symmetry of pore may be broken not only across (among x-direction) but also along the confining walls (among z-direction), which may change the phenomenon of capillary condensation much more subtle. Taking a semi-closed pore with finite depth w was an example (Fig.1b), the asymmetric effective forces acting from both ends of the pore on the liquid surface may smooth and shift the phase transition process, leading to a change from a first-order to a second-order phase transition. Researchers have proven that in a semi-finite slit, as the pressure (or chemical potential) increases, a single meniscus first forms at the sealed end, and then it gradually expands outward. This process is continuous, without sudden phase transitions, and therefore appears as a second-order phase transition. Therefore, studying only the phase behavior of fluids in parallel slit pores that maintain translational symmetry is not comprehensive.

In this paper, the phase behavior of hydrocarbon in nanopores formed of undulated pore walls is presented. Firstly, we present a purely macroscopic theory based on geometric arguments. This allows us to understand two possible capillary condensation mechanism in nano spaces. Then, the molecular simulation is conducted to capture the micro-structural evolution of confined hydrocarbon to determine the effect of adsorbed layers which the purely macroscopic theory neglects. The phase diagram also is drawled to illustrated the importance of geometric shape of nanopore.

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MS18 / 628

Sensitivity of soil representation in PFAS transport simulations under wetting and drying conditions

Author: Esther Cookson^{None}

Co-author: Russ Detwiler

Corresponding Authors: detwiler@uci.edu, cookson@uci.edu

Per- and polyfluoroalkyl substances (PFAS) can enter the vadose zone through episodic infiltration of surface waters, which ubiquitously contain these compounds. Elevated PFAS concentrations in shallow soils are primarily attributed to their accumulation at air-water interfaces, a phenomenon mostly studied near historical point source releases. Atmospheric conditions and infiltrating surface waters impact soil saturation in shallow soils, driving the expansion and contraction of air-water interfaces. Despite the recognized importance of these processes, the long-term impact of fluctuating soil saturation on the fate of PFAS in infiltrating surface waters remains poorly understood.

We simulated the retention and migration of perfluorooctanesulfonic acid (PFOS) from 15 years of periodic ponding of low-concentration (30 ng/L) surface water in a constructed wetland in the Santa Ana River watershed. We used Hydrus to model a 1D heterogeneous (sand-clay) system with boundary conditions informed by local surface water levels, precipitation, and evapotranspiration measurements. We also measured the grain size distribution of sediments from the field site. We used measured water retention curve parameters and permeability of sands and clays with similar texture and porosity to quantify the sensitivity of PFOS transport on soil properties (which are difficult to measure and often overlooked). Infiltration of surface water and atmospheric conditions drive changes in the saturation of shallow soils, which are mediated by soil physical properties. The resulting expansion and contraction of air-water interfaces redistribute PFAS within the pore matrix and control retention and migration of PFOS.

We considered two layering scenarios with the same effective saturated hydraulic conductivity (proportion of sand and clay). We observed differences in the total mass flux, distribution, and front propagation of PFOS for equivalent source concentrations, boundary conditions (precipitation, ponding, and evapotranspiration), and average permeability of the two scenarios. We found that some layered systems with shallow clay layers accumulate a greater mass of PFAS and develop persistently elevated pore water concentrations (up to four times the source concentrations) at shallow depths compared to corresponding layered systems with a top layer of sand. We evaluated multiple realizations of PFOS mass accumulation and will compare observations of the vertical distribution of PFAS in the field.

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Poster / 629

Quantifying low concentration in-situ field partitioning of PFAS in vadose zone sediments

Author: Esther Cookson^{None}

Co-authors: Ziwei Han ; Russ Detwiler ; Adeyemi Adeleye ¹

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Per- and polyfluoroalkyl substances (PFAS) are consistently detected in wastewater treatment plant effluent and urban stormwater runoff at concentrations that exceed federal health advisory levels. Soils and sediments in adjacent wetlands and floodplains may accumulate PFAS due to periodic ponding events. However, our understanding of PFAS transport and partitioning mechanisms in these areas is limited, particularly compared to well-studied sites with known point source releases and orders of magnitude higher concentrations. In this study, we measured the vertical distribution and solid-phase partitioning of perfluorooctanesulfonic acid (PFOS) in sediments collected from a wetland at the outlet of a large (5,0840 km²) urban watershed in semi-arid Southern California. The wetland is episodically ponded with water with some PFAS (e.g., recent PFOS measurements of 9 - 29 ng/l). Quantifying in-situ partitioning of PFAS in vadose zone soils requires knowledge of sorbed and aqueous phase concentrations and estimates of air-water interfacial areas. These are all difficult to measure directly in low permeability soils infiltrated with relatively low concentrations of PFAS.

We combined PFOS field sample measurements, laboratory batch desorption experiments, and partitioning models to quantify in-situ PFAS behavior in vadose zone soils. A batch desorption experiment on an interval directly below the field sample measured with the highest concentration of PFOS (6.53 ng/kg from 1.1 m depth) revealed that both a concentration-dependent Freundlich isotherm and a linear isotherm with an irreversibly adsorbed fraction (17% of the total in-situ mass of PFOS) fit the data well. We estimated in-situ partitioning by integrating the solid-phase partitioning isotherms with the air-water interfacial area and PFAS partitioning models. Pore-water concentrations estimated from a Freundlich air-water partitioning model were below 6 ng/L when paired with either of the solid-phase partitioning models. In contrast, pore-water concentrations estimated from a Langmuir air-water partitioning model ranged from 36.5 to 150.7 ng/L when paired with the linear solid-phase partitioning model, and from 3.9 to 218.7 ng/L when paired with the Freundlich solid-phase partitioning model. The wide range of predicted pore-water concentrations reflects uncertainties in sorption models and estimated air-water interfacial areas (varied by two orders of magnitude, even when constrained by grain size distribution). Finally, to assess possible hysteresis in soil-water partitioning, we performed adsorption/desorption/re-adsorption experiments on samples collected from 1.1 m, 1.9 m, and 2.8 m depths with varying fractions of organic matter and clay content. Mass-labeled PFOS were used to differentiate between field-exposed (PFOS), initial laboratory (M8PFOS), and secondary laboratory (M4PFOS) adsorption-desorption isotherms. This comprehensive study provides a sensitivity analysis of field measurements, partitioning mechanisms, and soil characterization models to evaluate the environmental fate and impact of common, low-concentration PFAS sources.

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MS18 / 631

Reconstructing historical PFAS concentrations in groundwater using a reduced-order modeling framework

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As the incidence of PFAS-contaminated drinking water increases around the world, understanding of sources and pathways of PFAS in complex urban watersheds continues to develop. In the Orange County groundwater basin in Southern California, recent sampling of over 500 monitoring and production wells has revealed concentrations of a group of PFAS compounds that exceed federal health advisory levels. As a result, dozens of production wells have been removed from service while treatment systems are being built. The groundwater basin is actively managed and recharged with surface water from the local Santa Ana River (SAR), imported surface water and purified recycled water. PFAS has recently been measured in the SAR at concentrations consistent with wells surrounding the recharge facilities suggesting that historic concentrations of PFAS in the SAR may be a primary input of PFAS in the groundwater basin.

Here we use an extensive set of PFOS, PFOA, PFNA, PFBS, PFHpA, and PFHxS groundwater concentration measurements from across the basin to reconstruct the water quality history of the SAR for each compound. We represent SAR-to-well transport using a reduced-order modeling approach. We develop transfer functions that describe transport along one-dimensional streamlines between each well and the likely source of recharge. We invert for the source history using truncated singular value decomposition. Dispersion coefficients and travel times to individual wells are determined by a hierarchy of models and data that include a calibrated MODFLOW model of the basin and a set of chloride breakthrough observations. Uncertainties in historical SAR concentrations are quantified by a Monte Carlo analysis that includes the uncertainty inherent in the required model parameters. We show that our reconstructed histories are in close agreement with recent measurements of PFAS in surface water from the SAR. We also combine the modeling framework with historical estimates of historical source concentrations to hindcast groundwater concentrations at production wells over the past 30 years. Estimated concentrations generally fall within the uncertainty bounds predicted by the Monte Carlo analysis. Our results may be helpful for estimating historical exposures and guiding investments in treatment facilities.

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MS26 / 632

Extensions to Early Work on Geologic Carbon Sequestration with Enhanced Gas Recovery (CSEGR)

Author: Curtis Oldenburg¹

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It has been 25 years since the first numerical simulation studies of Carbon Sequestration with Enhanced Gas Recovery (CSEGR) were carried out in the GEOSEQ project led by Sally M. Benson (Lawrence Berkeley National Laboratory). The early CSEGR simulation paper Oldenburg, Pruess, and Benson (2001) was followed by numerous studies and related publications on the subject by other researchers that continue to this day. Using the search terms “enhanced gas recovery’co2 carbon dioxide injection” in Google Scholar, one finds approximately 23 papers on the CSEGR topic prior to 2000, 130 papers between 2000-2005, 1101 papers for the decade ending 2015, and then 3400 additional papers for the decade ending in 2025 for a total of 4654 papers for the period 1985 to the present. This growth in publications after the year 2000 reflects both the rise of research in the field of geologic carbon sequestration of which Sally Benson is a respected pioneer and scientific leader, as well as the strong interest by industry in recovering natural gas from depleted reservoirs.

Since 2000, not only has the number of published studies in the area of CSEGR consistently increased, but so has the number of studies in tangential but very relevant topical areas that take advantage of the knowledge gained in CSEGR research and also the computational methods developed for it. For example, topics that have been addressed specifically but that are still of great ongoing interest because of their importance include: (1) effects such as deposition of impurities in CO₂ injectate, (2) challenges of CO₂ injection into low-pressure gas reservoirs, and (3) effects of gas composition on solubility and leakage attenuation. This talk will discuss these topics through presentation of simulation results and discussion of related implications for geologic carbon sequestration.

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MS26 / 635

Use of Synthetic Data for Designing Carbon Storage Strategies in Deep Saline Geologic Formations

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Model-based design tools will play a crucial role in the site selection, design, and safe operation of carbon storage facilities within deep saline formations. When selecting sites, key factors such as the permanence of storage through stable trapping and mineralization must be considered. The design process involves strategic decisions regarding injection placement and timing. Ensuring safe operation entails addressing potential leakage of stored CO₂ and the formation brine, which can arise from pressure build-up that may fracture the caprock or reactivate existing faults. These issues pose a risk of contaminating shallow aquifers used for drinking water and other economic activities. To effectively characterize sites, comprehensive data on the expected geologic conditions is essential. Continuous monitoring is also required during operation to detect any potential leakage events and if such an event occurs how to reduce the risk of shallow aquifer contamination. The significant depths of these formations create numerous technical challenges and cost constraints in gathering relevant geological information and monitoring data. As leakage events have not yet been observed at existing sites (primarily during pilot testing), there is currently a lack of data to validate the models necessary for effective carbon storage design.

In this paper, we present an approach utilizing an intermediate-scale test system to test and validate numerical modeling tools. The term “intermediate scale” refers to a dimension where multi-dimensional experiments can be conducted to simulate field conditions. This allows for the generation of accurate spatial and temporal data based on well-defined soil packing configurations that account for heterogeneity under known initial and controlled boundary conditions. The data generated through these experiments was utilized to validate models that produced synthetic data for analyzing the effects of geological uncertainties in the storage zone, fracture configurations in the caprock, the aquifer zone above the caprock, and the shallow aquifer. We discuss how this data can be leveraged to develop optimized monitoring systems that rely on fewer deep zone data while utilizing more readily available shallow zone data. Additionally, we present examples of remediation strategies involving pressure release in the storage zone

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MS26 / 637

Rapid Field-Scale CO₂ Storage Simulation tool with Geomechanically constrained Fault Leakage function to Predict Leakage Outcomes under Uncertainty

Author: Hariharan Ramachandran¹

Co-authors: Ikhwanul Hafizi Musa²; Chee Phuat Tan³; Sebastian Geiger ; Florian Doster

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Storing CO₂ in geological formations is a crucial method for mitigating climate change. However, CO₂ leakage poses a threat, with faults representing a significant concern. Accurately simulating

fault at different scales is crucial to predict the consequences of CO₂ injection and storage at the field-scale. However, this task can be challenging, particularly in the early stages of a storage project since 1) knowledge of the storage reservoir is limited, 2) Obtaining high-quality well logs, cores, and seismic data is expensive, and 3) Resolving the impact of fine-scale fault features on field-scale storage assessment is computationally expensive.

This study proposes a fast tool for CO₂ leakage risk assessment that addresses these challenges at both the project screening stage and advanced stages of project planning. The tool uses a vertically integrated reservoir model coupled with an upscaled fault leakage function based on source/sink relations. The fault is conceptualized as an increased vertical permeability through the caprock (due to the fracture network in the fault damage zone) and a reduced horizontal permeability through the reservoir (due to fault throw and fault core). A steady-state flow approximation is used to estimate CO₂ leakage along the fault. Certain fault properties are geomechanically constrained to reflect the impact of pressure changes within the reservoir-caprock system. Geomechanical effects on fluid flow are modeled by relating porosity, permeability amongst several other parameters to effective stress using constitutive relations.

This study presents results validating the fault leakage function using 3D reservoir simulations. Example simulations are also shown to illustrate 1) impact of fault leakage on storage capacity, 2) impact of geomechanically constrained fault parameters such as capillary entry pressure and permeability on fault leakage for an example storage site located within Malay Basin. The fast model presented in this study is a valuable tool for identifying uncertainties in key fault parameters and other constitutive relations that affect the behavior of the storage reservoir and potential fault leakage outcomes. By incorporating this tool into the site screening stage, stakeholders can quickly assess the risk of CO₂ leakage and evaluate the feasibility of the storage site under wide range of injection conditions.

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MS03 / 643

Experimental validation of a graph-based model to represent colloid transport and fracture-matrix transport processes

Author: Collin Sutton¹

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Fractures are voids in rock, defined by rough surfaces in partial contact, that often create complex flow and transport networks. Flow and transport in fractured systems is complicated by coupled processes such as colloid transport, water-rock interactions, and geomechanics. Understanding these coupled processes is essential for permeability and injectivity management in oil and gas operations, carbon dioxide injection, geothermal reservoirs, and managed aquifer recharge. Despite the significance of fractured systems, challenges persist in quantifying coupled transport processes given the opaque nature of rocks and limitations of traditional experimental techniques. This study overcomes these challenges by using a combination of pulse-tracer experiments with positron emission tomography (PET) and reduced physics flow and transport models to characterize (1) colloid transport and

(2) fracture-matrix interactions in rock cores with mechanically generated fractures.

In the first set of experiments an aqueous pulse of suspended radiolabeled kaolinite ($^{64}\text{Cu}^{2+}$) is injected into a 5.08 cm diameter fractured Sierra granite core under single-phase flow conditions. Flow-through experiments are conducted under varying flow rates to evaluate hydrodynamic effects on colloid retention and breakthrough behavior. A second set of experiments was performed that use a conservative radiotracer (^{18}F -FDG) injected into a 5.08 cm diameter fractured Berea sandstone core under single-phase flow conditions. Berea sandstone is used because it has high matrix porosity and allows for the quantification of solute transport through both matrix and fracture. Simultaneous PET imaging during both experiments allows for high-resolution, in-situ visualization and quantification of solute and colloid distributions at the millimeter scale.

The PET imaging experiments provide spatially resolved data and traditional coreflooding provides bulk-scale breakthrough, enabling the testing for reduced-physics models to accurately capture coupled flow and transport processes in fractured rock. Prior work has shown that graph-based, random-walk particle tracking techniques accurately model conservative solute transport in fractured cores (Sutton & Zahasky, 2025). Here, that algorithm is modified based on first-order kinetics (Liu et al., 2022) and is used for colloid transport and diffusion into a porous matrix. The model is validated against experimental data, demonstrating its ability to characterize colloid tailing behavior and attachment dynamics as well as transport in a fracture with adjacent porous matrix. This work demonstrates that graph-based modeling of fractures can effectively capture complex processes, offering computationally efficient modeling approaches without requiring explicit geometric definitions. While previous studies have shown that graph-based approaches accurately quantify conservative solute transport in a single fracture, this is one of the first studies to validate this modeling approach for coupled transport processes.

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References:

Sutton, C. R., and C. Zahasky (2025), A laboratory-validated, graph-based flow and transport model for naturally fractured media, *Geophysical Research Letters*, 52, e2024GL112277, <https://doi.org/10.1029/2024GL112277>.
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644

Three-dimensional digital characterization and mechanical properties analysis of rock cuttings

Author: Huaimin Dong¹

Co-authors: Lezi Wang²; Bidong Zhang²; Likai Cui³

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Digital quantitative rock analysis technology enables the non-destructive and quantitative evaluation of minute quantity rock samples. As a cutting-edge technology in the oil and gas sector, which can offer convenience, speed, precision, and cost-effectiveness, and provide valuable insights for reservoir positioning and simulated enhanced oil recovery techniques, thereby supporting informed decision-making in oil field exploration and development. The cuttings are the real data from the stratum and have the characteristics of continuity and real-time. The effective use and analysis of cuttings samples have an important impact on oil and gas identification, formation correlation and later interpretation and evaluation at the well logging site. However, high speed drilling results in more and more fine cuttings, and limited by analytical equipment and methods, there are many difficulties in quantitative analysis. This study is based on detection methods such as X-ray diffraction, elemental analysis and micron CT scanning, systematically analyzed the lithology and porosity range of the strata represented by cuttings, and carried out multi-stage and multi-scale screening of the collected cutting samples to conduct multi-sample CT scanning. By matching Qemscan images and CT scanning images, multi-component and multi-scale three-dimensional digital rock models were constructed. Through comparing the porosity and permeability parameters, the accuracy of the digital rock model is confirmed, and based on this model, the numerical simulation of rock physical characteristics is carried out to realize the quantitative analysis of formation rock mechanics and other parameters.

Country:

China

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Water & Porous Media Focused Abstracts:

References:

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645

Discrete modeling of limestone particle calcination under non-isothermal conditions

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In this study, we develop a discrete model based on pore network modeling to simulate heat transfer, mass transfer, chemical reactions, and fluid-solid interactions during the calcination of a single limestone particle under realistic non-isothermal conditions. This model differs from our previous work by capturing internal temperature distributions through local energy equations. It also systematically updates the sizes of solid grains and pore structures over time, accurately reflecting

the evolution of local conversion profiles, pore size distributions, and internal temperature fields. Temperature gradients in the particle cause a non-uniform release and transport of CO₂ to the surrounding environment. In certain pore regions, CO₂ pressures exceed equilibrium levels, leading to clogging of the pores. Such insights are crucial for the proper development of single particle continuum models that can more accurately mimic the realistic conditions of the calcination process.

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Flow of liquid foam through porous media

Author: Ali Salame¹

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Due to the human activity of enhanced oil recovery, foam transport in porous media is a huge field of investigation. In processes where gas (usually steam, carbon dioxide or hydrocarbon gas) is injected into an oil field to improve oil recovery, foam can help divert gas into untouched portions of the reservoir. More recently, foam is used in soils for improvement or remediation purposes. In these applications, it is important to anticipate how far from the injection point foam can be transported, and to know the relative permeabilities of both gas and liquid. Although scientists in the field have some knowledge about bubbles interactions within the pore-space of the rocks, for example, to predict the effective yield stress of the transported foam, the microstructure of the foam is far from being understood.

Here, we show results regarding the flow of liquid foam into the porosity of granular packings. Rheological curves are derived from pressure-flow relations and will be presented as a function of bubble size, grain size, and liquid saturation. We highlight that, to accurately understand foam rheology in porous media, it is essential to halt bubble coarsening, the gas-driven pressure phenomenon responsible for bubble size increase over time. We show that confinement effects of foam flow through granular packing cannot be directly extrapolated from bulk foam properties. Instead, it is primarily governed by the degree of confinement, represented by the bubble-to-grain size ratio. We observed a progressive increase in the confined foam's yield stress as confinement intensified. Results for the flow of complex liquid foams, i.e. liquid foams loaded with solid particles, will be considered.

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Water & Porous Media Focused Abstracts:**References:**

O. Pitois, A. Salamé, Y. Khidas, M. Ceccaldi, V. Langlois, and S. Vincent-Bonnieu, 'Daisy-shaped liquid bridges in foam-filled granular packings', J. Colloid Interface Sci., vol. 638, May 2023, doi: 10.1016/j.jcis.2023.01.127.

Poster / 650

The efficacy of heat sensitive epoxy foam for permeability alteration in fractured geothermal fields –Laboratory experiments

Authors: Cui Yutong¹; Rishi Parashar^{None}; Manish Bishwokarma^{None}; Ying Yang^{None}; Satish Karra^{None}; Dani Or²

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Geothermal energy plays an important role in the transition towards renewable and carbon-neutral energy resources. For some geothermal fields enhancing water-rock heat exchange is required by either fracking or by blocking large conduits. Here we test a novel approach for blocking large fractures using heat sensitive epoxy resin foam droplets that can be advected to target regions of the geothermal and then thermally activated to foam (release CO₂) and simultaneously cure to create obstacles and reduce local permeability. Laboratory experiments using aluminum-glass fracture models provide insights into the process by visualizing resin droplet transport and subsequent temperature-induced foaming and curing that visually show pathway blocking and reduced permeability. A conceptual model for flow and transport of droplet swarms in single fracture is developed to illustrate how aperture modifications affect upstream pressure, flow pathways and permeability.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:****Poster / 651**

Identification of Hydraulic Backbones in Discrete Fracture Networks with Genetic Algorithms and Localized Graph Contraction

Author: Ryan "Emmy" Shaver¹

Co-authors: George Bebis ²; Rishi Parashar ¹

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Discrete fracture networks (DFNs) offer high-fidelity simulations of flow and transport in fractured media, but the complex networks they represent are often computationally prohibitive at field scales. Identification of network backbones, relatively small subgraphs that capture major network processes, can significantly reduce computations and expose important topological structures. We introduce a novel method for identifying hydraulic backbones in DFNs using genetic algorithms and localized graph contractions. In contrast to previous work identifying backbones where major transport processes occur, our work provides network simplification further upstream in the DFN methodology, identifying major hydraulic processes and potentially reducing downstream computations. To ensure backbone connectivity, we use a path-based search space. Otherwise prohibitively vast, we introduce an on-the-fly search space reduction technique based on localized graph contractions that utilize fracture networks' fractal-like structure. Unlike prior machine learning-based identification methods that may require extensive offline training, we use a genetic algorithm for backbone identification that requires no training, at the cost of longer prediction times. Our methodology is tested on 27 synthetically generated DFNs of varying heterogeneities, and one DFN imaged from actual fractured rock. We quantitatively measure backbone validity with the size reduction gained by the subgraph, along with how well it mimics the original network's conductivity tensor and flow velocity distribution. Qualitative inspection of identified backbone and non-backbone regions reveals hydraulic structures vital to downstream flow and transport simulations, as well as less hydraulically important structures that may be simplified or omitted altogether.

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Poster / 652

Transport of plant-based and enteric viruses in homogenous saturated porous media

Author: Emmanuel Cobbinah¹

Co-authors: Lin Li ²; Subhash Verma ³; Krishna Pagilla ²; Todd G. Caldwell ⁴; Rishi Parashar ⁵

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Water reclamation and reuse has become a popular practice in arid to semi-arid regions, especially in the western United States. Conventional wastewater treatment methods often fall short of completely removing viruses, causing the introduction of myriad of viruses in the water environment with potential for hazardous impact on human health. Current fecal contamination indicators including *Escherichia coli* and coliform bacteria, showing high seasonal variations in their concentration, do not exhibit any significant relationships with enteric viruses in the wastewater. Plant-based viruses occur at consistently high concentrations in the wastewater—however few studies have explored their potential to be surrogates for tracking of enteric viruses in water reclamation systems. Using uniform diameter glass beads to construct homogenous columns, we conducted experiments to investigate the transport behavior of Pepper Mild Mottle Virus (PMMoV), Tomato Brown Rugose Fruit Virus (ToBRFV), and human adenovirus (hAdV) under saturated conditions. After injecting wastewater for four pore-volumes, the columns were flushed with dechlorinated tap water for an additional six pore-volumes, Column effluents were enumerated using reverse transcription quantitative polymerase chain reaction (RT-qPCR) and analyzed using advection-dispersion-reaction models. Our results indicated a similar transport behavior for the ToBRFV and PMMoV marked by steep rising limb and a heavy-tailed breakthrough curve, whereas hAdV showed a significantly milder rising limb. These observations were examined by drawing insights from Derjaguin–Landau–Verwey–Overbeek (DLVO) theory and physical attributes of viruses. In addition to identifying potential surrogates for enteric viruses in water environment, this study is a step towards upscaling and extrapolating of virus transport dynamics in water reclamation systems for sustainable water reuse

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653

Evaluation of Transfer Learning Models for Upscaling Pore Scale Properties

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Co-authors: Hongkyu Yoon²; Sanghyun Lee³; Son-Young Yi¹; Soumya Shouvik Bhattacharjee¹; Zhengtao Gan⁴

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Accurate upscaling of the porous media properties is very important in science and engineering fields for various applications such as geothermal energy extraction, geologic carbon/hydrogen storage, oil reservoir analysis, and material design. While pore-scale simulations provide detailed insights, they are computationally expensive. Over the past few years machine learning approaches,

particularly Convolutional Neural Networks (CNNs), have emerged as promising alternatives for upscaling. However, traditional CNN-based methods require extensive training data and/or extensive retraining when new data is introduced. On the other hand, transfer learning methods use pre-trained weights and biases and do not require a lot of data to train. Also, it requires a relatively short time to train, compared to training traditional CNN-based models. Moreover, we can introduce different kinds of new required geometric configurations even after retraining without facing severe catastrophic forgetting issues. However, these methods have not been widely explored yet in upscaling tasks. In this study, we will try to explore the capabilities of transfer learning models like Swin Transformer, ResNet, DenseNet, and Inception with the integration of different configurations of pore geometries. We will try to map 2D porous media images of a specific range of porosities to their corresponding permeabilities and examine the performance of already mentioned methods based on their efficiency and accuracy and then compare them with traditional CNN-based architectures.

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Poster / 654

Numerical parametric analysis of Triply Periodic Minimal Surfaces with deep learning

Authors: Eleonora Gajetti¹; Gianluca Boccardo²; Agnese Marcato³; Luca Marocco⁴; Laura Savoldi²

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Triply Periodic Minimal Surfaces (TPMS) have been gaining interest in recent years as structured porous medium in numerous engineering applications [1](#), including compact heat exchangers [2](#), [3](#), [4](#), heat sinks [5](#) and phase change materials [6](#). TPMS are periodic lattices generated by the combination of sine and cosine functions in 3D, the manufacturing of which has been enabled by the deployment of Additive Manufacturing (AM) techniques. TPMS have large surface-to-volume ratio and no sharp edges, which enable high heat transfer efficiency, while simultaneously maintaining the pressure drops low. Different combinations of trigonometric functions may lead to different characteristic equations thus several diverse topologies, featuring widely disparate properties. Furthermore, TPMS performance depends heavily on their geometric parameters, such as porosity, cell size or cell orientation. Therefore, TPMS can be adapted to the different engineering problems, and optimized according to the constraints they must comply with.

Although many research studies on TPMS, both thermal and hydraulic, can be found in the literature, there is a lack of comprehensive and structured parametric analysis of the impact of their constitutive geometrical parameters, as can be achieved using deep learning. The present work aims at bridging this gap, investigating thoroughly the effects on the pressure drop of the porosity and

cell orientation. In view of the very large parameter space which could be explored, to make the investigation feasible, a deep learning technique consisting in artificial neural network is adopted. Numerous CFD simulations are first performed on a single periodic lattice cell for different topologies, to calculate the flow field with Reynold number in the range 1-150, considering a wide range of porosity values and orientation angles of the lattice. Part of the numerical results, in terms of pressure drop, is used as the database for training a neural network (NN), suitably tailored for the purpose. The NN is tested on a subset of the CFD results not used for the network training, showing an excellent capability to foresee the lattice cell hydraulic characteristics. It is shown that the developed surrogate model can be used, for instance, as a selection tool for the best configuration (in terms of topology, porosity, orientation) when the minimum pressure drop is prescribed and the mass flow rate in the lattice is targeted.

¹ M. G. Gado et al., Energy Technology, May 2024

² T. Dixit et al., Appl Therm Eng, Jun. 2022

[3] B. W. Reynolds et al., Int J Heat Mass Transf, Sep. 2023

[4] D. Liang et al., Int J Heat Mass Transf, Feb. 2023

[5] N. Baobaid et al., Case Studies in Thermal Engineering, May 2022

[6] Z. A. Qureshi et al., International Journal of Thermal Sciences, Mar. 2022

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655

Advancements in Hierarchically Structured Porous Materials for Enhanced Mass Transport in Cleantech Applications

Author: Milana Trifkovic^{None}

Co-authors: Markus Lee ¹; Keenan Smith ²; Fabrizia Foglia ²; Abdul Mansoor Basha ¹; Kunal Karan ¹

¹ University of Calgary

² University College London

Corresponding Authors: keenan.smith.18@ucl.ac.uk, mtrifkov@ucalgary.ca, kkaran@ucalgary.ca, abdulbashith.mansoor@ucalgary.ca, f.foglia@ucl.ac.uk, minhyung.lee1@ucalgary.ca

Fluid-fluid interfaces containing nanoparticles offer a versatile platform for creating hierarchically structured materials with tailored properties. In this study, spinodal decomposition is employed for the first time as a template for fabricating catalyst layers (CLs) in proton exchange membrane fuel cells. By leveraging the phase separation of water/2,6-lutidine mixtures, this approach generates hierarchical pore structures, introducing a novel pathway for CL design.

The structural evolution of these catalyst inks was investigated using a multiscale approach, integrating small-angle neutron scattering (SANS), microrheology, bulk rheology, and fuel cell performance testing. At the critical composition of the water/2,6-lutidine mixture (72:28 wt%), ionomer chains

were found to adopt a compact conformation with a higher overlap concentration compared to conventional alcohol-based media. During spinodal decomposition, SANS revealed the formation of large-scale ionomer chain clusters induced by the low dielectric constant of lutidine. However, in the presence of carbon-supported platinum (Pt/C) catalyst particles, ionomer cluster formation was suppressed due to spatial confinement during the water/lutidine phase separation and enhanced ionomer-catalyst interactions.

Microrheology revealed a significant contrast in ionomer-Pt/C interactions between the miscible state of water and 2,6-lutidine (at room temperature) and the phase-separated state (above the lower critical solution temperature of 34°C). These interactions intensified notably during phase separation, anchoring the ionomer chains to the Pt/C surface. Bulk rheological measurements further captured the development of robust percolated networks during spinodal decomposition, which preserved their structural integrity during the drying process.

Fuel cell performance testing demonstrated that spinodally decomposed CLs outperformed conventionally prepared CLs in the mass-transport-controlled high current density region. This improvement is attributed to the larger pore structures and interconnected networks observed in SEM imaging, which enable more efficient mass transport and improved ionomer-Pt/C contact.

These findings establish spinodal decomposition as a powerful tool for fabricating hierarchically structured CLs. By offering new insights into ionomer chain behavior, catalyst interactions, and hierarchical structuring, this approach paves the way for optimizing material architectures in energy conversion technologies, particularly proton exchange membrane fuel cells.

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References:

MS22 / 656

A Density Functional Theory-based Force Field for Modelling Silica-Water Interfaces

Author: Jeffery Greathouse¹

Co-authors: Sahan Godahewa²; Thanuja Jayawardena²; Ward Thompson²

¹ Sandia National Laboratories

² University of Kansas

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The silica-water interface is well studied given its ubiquity in geochemical environments. Many force fields have been developed for both silica and water independently, however, little attention has been given to interaction parameters developed specifically for the interface. As a consequence, simulations continue to use traditional “mixing rules” to calculate silica-water Lennard-Jones interaction parameters. This study bridges this gap by developing a force field explicitly optimized for silica-water interfaces beyond mixing rules. Silica-DDEC, a recently developed force field with electrostatics matched to density functional theory (DFT) is used as the starting point. Lennard-Jones parameters are developed by benchmarking against DFT-derived interaction energies. The results reveal that traditional mixing rules overestimate water binding energies while the new parameters

correct this error for β -cristobalite and amorphous silica surfaces. The parameters are also transferable to other silica interfaces such as α -quartz. The performance of the new parameters is further investigated for its effect on the structural and dynamic properties of water in silica slit pores. The improved parameters lead to faster dynamics due to the elimination of the overbinding effect. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS12 / 657

Finite volume methods for poromechanics

Authors: Jan Martin Nordbotten¹; Eirik Keilegavlen¹; Wietse Boon^{None}

¹ *University of Bergen*

Corresponding Authors: eirik.keilegavlen@uib.no, jan.nordbotten@math.uib.no, wibo@norceresearch.no

In this talk, we survey recent advances in finite-volume type discretizations for mechanics and poromechanics. We will in particular discuss three classes of discretizations. 1) Multi-point stress finite volume methods (MPSA). 2) Two-point stress finite volume methods (TPSA). 3) Multi-point stress mixed finite element methods (MSMFE).

Being finite volume methods, the three classes of methods mentioned provide numerical approximations that have explicit flux and stress expressions, and where these fluxes and stresses balance exactly with the right-hand side of the equations. However, their different construction leads to both qualitative and quantitative differences.

We will provide a brief overview of the philosophy between each class of methods, and systematically address their strengths and weaknesses. Our qualitative discussion will emphasize the generality of the methods in terms of grids, non-linearities, generalizability, and robustness in terms of degenerate parameters that are relevant in applications.

We will also survey more quantitatively the relative performance of the methods on a set of test cases.

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658

Effects of lamina combination on physical properties of shale samples based on 3D multimineral digital rocks

Authors: Yuqi Wu^{None}; Jiabao Yang¹; Yuchen Fan^{None}; Keyu Liu¹; Sheng Zou¹

¹ *China University of Petroleum (East China)*

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Shale samples are extremely heterogeneous and they not only involve the multiscale pore systems and multiple-type minerals, but they also contain various horizontal laminae. Different laminae consist of distinct minerals, organic matter, and pore systems. The lamina type, volume fraction, and frequency could affect the physical properties of the whole shale sample. However, it is difficult to quantitatively analyze the relationship between the rock properties and lamina type and volume fraction by only using experimental techniques since the laminae are extremely thin, smaller than one millimeter in thickness. Therefore, the digital rock technique, as a robust tool, is used to achieve such a goal by virtue of the flexibility of 3D digital models. The first step for this aim is to construct a set of 3D digital rocks containing various laminasets. Thus, we combine the Advanced Mineral Identification and Characterization System (AMICS), Multiple-Point Statistics (MPS) method, and image processing algorithm to build 3D digital models of many laminasets. Herein, AMICS is used to precisely identify the mineral types in 2D scanning electron microscopy images, and the MPS algorithm is utilized to reconstruct 3D multimineral digital models of different laminae based on 2D training images. The mineral and pore properties of the produced 3D digital models are validated to be in good agreement with those of 2D training images. Furthermore, the 3D digital models of two and three laminae are superposed together to generate 3D digital rocks with different laminasets. Based on 3D laminated digital rocks, the effects of the lamina type and volume fraction on porosity, pore tortuosity, fractal dimension, and permeability of shale samples are comprehensively analyzed. The results reveal that the felsic mineral lamina could enhance the shale porosity, fractal dimension, and permeability and the increase in the organic matter lamina leads to the reduction in these petrophysical properties. The increase in the carbonate mineral lamina results in the surge of the bulk modulus and shear modulus of the shale sample. The variation degree of those petrophysical properties also depends on the original fractions of the laminae. Moreover, the porosity, fractal dimension, permeability, and elastic moduli of the felsic-mineral-carbonate-mineral laminaset are the highest and its pore tortuosity is the lowest among all the laminasets. By contrast, the organic-matter-clay-mineral laminaset presents the lowest porosity, fractal dimension, permeability, and elastic moduli. Consequently, it is critical to select the optimal laminated shale layer for the next development of the shale oil.

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MS14 / 659

Uncertainty quantification for reactive transport in random porous media

Authors: Nikolay Shegunov¹; Oleg Iliev^{None}; Petar Armyanov¹

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In this work a problem that describes a reactive transport inside a random porous medium is considered. The main driving force of the transport is the processes of convection and diffusion, which are influencing the reaction. This type of simulations has practical applications in oil recovery, soil pollution and remediation, as well as in several industrial and biomedical processes.

A steady-state two-dimensional convection-reaction-diffusion equation with random coefficients is considered. It describes reactive transport in random porous media consisting of sand, gravel, and other soils. The equation is considered in its dimensionless form. The applicability and superiority of MLMC method for solving such problems with a huge parametric space is demonstrated. The coarse grain strategies used for constructing the MLMC model are discussed. Lognormal distribution of the permeability is considered, based on numerous experimental observations. Essential part of the algorithm is the fact that the random coefficients for the flow problem and for the reactive transport are not independent. In fact, random coefficients are generated for the flow problem, and using them coefficients for the reactive transport are derived based on the standard models for flows in porous media and heterogeneous reactions.

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Poster / 660

Enhanced Wellbore Integrity Through Pumice-Modified Cement Systems: A Novel Approach for Hydrogen Storage Applications

Author: Leonard Kobina Asare^{None}

Co-authors: Franklin Duodu Ahwireng¹; Rexford Donkor¹

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This research investigates the application of pumice-modified cement systems in improving wellbore integrity for hydrogen storage wells. Laboratory experiments conducted on cement compositions containing 5-25% pumice by weight demonstrated significant improvements in both mechanical properties and gas containment capabilities. The optimal blend (15% pumice) exhibited a 40% reduction in gas migration along the cement-casing interface and a 35% increase in bond strength

compared to conventional cement systems. Under simulated downhole conditions (75°C, 150 bar), the modified system showed remarkable resistance to temperature-induced stress cycling, maintaining structural integrity after 100 thermal cycles (25-75°C). Microstructural analysis revealed that pumice addition created a refined pore network that enhanced cement-formation bonding while reducing permeability. Notably, the system demonstrated superior resistance to hydrogen-induced degradation, with only a 2% strength reduction after 6 months of exposure to hydrogen at storage conditions. These findings provide crucial insights for designing more reliable wellbore barrier systems in hydrogen storage applications, particularly in preventing gas leakage and maintaining long-term well integrity.

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Plenary Lecture / 662

Safe and Efficient CO₂ Sequestration in Subsurface Aquifers: Viscosity Enhancement, Physics of Displacement, and Numerical Modeling

Author: Abbas Firoozabadi¹

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CO₂ has gas like viscosity and liquid-like density. Injection in the subsurface results in wide distribution and possibility of leakage. Direct viscosification of CO₂ at low concentration requires engineering of new molecules that can be effective in the subsurface conditions. The phase behavior description of water/brine and CO₂ is still an unresolved issue. Advances are being made for accurate and efficient phase behavior description. Phase behavior computations have been recently advanced for large scale simulations.

The physics of flow of water/brine and CO₂ has complexities that have not been recognized until recently. In most publications, the capillary pressure is assumed to be zero at the core outlet in lab scale. Recent X-ray CT scanning shows the boundary conditions even in Lab scale may be revisited. The most challenging problem has been large scale flow simulations. When CO₂ dissolves in water/brine, there is density increase. Gravity fingers develop from adverse density effects. Most large-scale flow simulators cannot capture the gravity fingering properly. The domain discretization by 3D fully unstructured gridding, and higher-order methods have been recently integrated in dynamic adaptive gridding.

The presentation combines recent advances in various aspects of the problem leading to large scale modeling of CO₂ sequestration in subsurface aquifers.

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References:**Plenary Lecture / 664****Flow architectures in porous media, designing for efficiency**

Author: Sylvie Lorente^{None}

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Flow systems can evolve toward greater efficiency by adapting, or ‘morphing’, their configuration to decrease flow resistance. Flow channels function in concert with the structures around them, as a combination of long and fast flows along the channels, with short and slow flows through the surrounding medium. The ability to predict flow patterns enables engineers to propose flow designs for heat, mass, and fluid flows. Our previous work theorized the deterministic nature of morphing and showed how to obtain efficient flow configurations for combined and sometimes competing objectives.

In this talk we will consider applications ranging from the control of ionic species transport, energy storage based on thermochemical reactions and the design of capillary networks for the cooling of high-power electronic components.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:****Plenary Lecture / 665****The love story between particle porosity and the biomedical field.**

Author: Achraf Nouredine¹

¹ *University of New Mexico - Chemical and Biological Engineering*

Corresponding Author: anouredine@unm.edu

Engineering material porosity was initiated to harness their properties in catalysis and separation. Shortly after, adapting porosity to nanotechnology was embraced by the biomedical field: Particle porosity not only can accommodate, concentrate and protect nanocatalysts or nanotherapeutics from small molecule drugs to nucleic acids and proteins, but we have found that they also exhibit

intrinsic properties that guide the interaction of the nanomaterials within their biological environment, including cell lipid membrane, uptake, biocompatibility, particle dissolution, but also to some extent their distribution in body organs. In this presentation we will first revise the basics of pore formation within silica matrices, their interaction with therapeutics and selected works by our group in bio- and catalytic applications of porous silica materials.

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Invited Lecture / 667

Water transport through hygroscopic porous materials (paper, wood, textiles, fiber panels): a subtle three-phase flow

Author: Philippe Coussot¹

¹ *Univ. Paris-Est*

Corresponding Author: philippe.coussot@ifsttar.fr

Most bio-based materials, such as paper, natural textiles, sponges, wood or plants, fiber panels for insulation, are porous systems through which water transfers play an essential role in the applications. A specificity of these materials is that they are also hygroscopic: they can absorb huge amounts of water, typically up to about 25% of their dry mass, from ambient vapor, in the form of bound water confined at a nanoscale in the amorphous regions of the cellulose structure, a bound water at the origin of the significant swelling of these materials. Remarkably, this bound water is also strongly mobile inside the solid phase. For example, the bound water contained in a cellulose fiber stack whose porosity has been filled with oil may be extracted by drying, proving that it is transported inside the fibers throughout the network. Moreover, the corresponding transport diffusion coefficient of bound water appears to be rather large, in the order of the self-diffusion coefficient of (free) water. These characteristics imply that, more generally, in hygroscopic porous materials, water can be transported through the system in three different phases, i.e., vapor, free water and bound water, which are strongly coupled via sorption or desorption processes. Finally, the coupling between some or all of these different processes leads to unexpected physical characteristics.

The original implications are illustrated by the long-term evolution of an aqueous droplet, possibly containing particles such as pigments and viruses or solute such as ions and polymers, and reaching the surface of a cellulosic sample. It is generally considered that such a droplet somewhat spreads, penetrates the structure, stabilizes and eventually dries. In fact, it may be shown from NMR (nuclear magnetic resonance) relaxometry and MRI (magnetic resonance imaging) that, instead of drying, the water is absorbed as bound water and diffuses throughout the entire structure. Thus, the initial (free) water rapidly disappears from the porosity, while the non-absorbed solute or particles remain stuck to the solid surfaces in the initial region of liquid penetration.

Another original effect is the imbibition of wood with water. As observed with NMR and MRI, the standard liquid water penetration thanks to capillary effects through vessels is slowed down by several orders of magnitude of time because the structure does not allow the invasion of free water in the regions where cell walls are not saturated with bound water.

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References:**Invited Lecture / 668**

Phase-field modeling for multiphase flow and geomechanical processes

Author: Luis Cueto-Felgueroso¹

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Phase-field models have proven to be effective simulation tools for describing interfacial processes at computationally feasible scales. Recent applications of these models include simulating the nucleation and propagation of hydraulic fractures in geological formations, as well as the behavior of fluid-fluid interfaces during flow through permeable media. The phase-field approach seeks to upscale interface dynamics by developing a continuum representation that diffuses sharp interfaces across several grid blocks or elements within a computational mesh.

The governing equations are formulated using appropriate variational principles or thermodynamic descriptions of the system. In this work, we present a phase-field formulation for thermo-hydro-mechanical hydraulic fracturing, with applications in geothermal energy production, and in the migration and seafloor venting of hydrocarbons. Additionally, we introduce a fugacity-based phase-field model for multiphase, multicomponent flows, applied to pore-scale simulations in the context of CO₂ and hydrogen storage in porous formations. We also address the challenges of bridging scales in these models.

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The Influence of Multiple Scales in Fractured Media on Flow and Transport Properties

Author: Jeffrey Hyman¹

¹ *Los Alamos National Laboratory*

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In low-permeability fractured media, such as granites and shales, flow and the associated transport of dissolved solutes is controlled primarily by fractures embedded within the rock matrix. The geometry of individual fractures, size and aperture, as well as the network structure determine the structure of the fluid flow field. However, the relevant lengths scales within a fracture network range several orders of magnitude and it is unclear which features of the network influence which flow and transport properties. One tool to investigate the interplay and influence of these multiple scales are discrete fracture network (DFN) models. In this talk, I'll discuss recent studies that use high-fidelity DFN models that attempt to link flow and transport attributes to physical structures of a fracture network ranging in-fracture aperture variability to network-scale connectivity.

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Invited Lecture / 671

Reactive transport processes in porous rock sample: role of local heterogeneities.

Author: Linda Luquot¹

¹ *CNRS-Géosciences Montpellier*

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The percolation of acidic fluids through natural rocks (e.g. CO₂ storage, Karst formation, geothermal formation) induces chemical reactions of dissolution and/or precipitation, which consequently alter the structural and hydrodynamic properties of the rock. These reactions are not uniformly distributed but instead become localized based on various local parameters, such as fluid velocity heterogeneities, chemical or mineralogical composition, and petrophysical properties. Understanding the influence of these local heterogeneities is crucial for predicting the evolution of rock properties in natural and engineered systems.

This study presents laboratory experiments involving the percolation of reactive fluids through rock samples. The primary objective is to elucidate the role of local heterogeneities in governing reaction rates, the type of reactions occurring, their spatial localization, and the resultant impacts on structural and hydrodynamic properties. The experiments are designed to simulate natural conditions, allowing for controlled variations in fluid flow rates, chemical composition, and rock mineralogy. Key findings from these experiments reveal that local variations in fluid velocity significantly influence the distribution and intensity of dissolution and precipitation reactions. Zones of higher fluid velocity tend to exhibit more pronounced dissolution due to increased fluid-rock interaction time and reactant supply. Conversely, areas with slower fluid movement often show precipitation as a result of reactant saturation and limited transport away from the reaction sites. Chemical composition and mineralogical heterogeneity further modulate the reactions. Petrophysical properties, such as porosity and permeability, also play a critical role. High-porosity regions facilitate fluid flow and enhance reaction rates, whereas low-porosity areas impede fluid movement, reducing reaction rates. These variations result in differential alterations in rock properties, creating a heterogeneous structure that affects overall permeability and fluid flow patterns.

The results underscore the complexity of fluid-rock interactions in heterogeneous systems. They highlight the importance of considering local heterogeneities when predicting the behavior of natural and engineered systems subjected to reactive fluid percolation. The insights gained from these laboratory experiments contribute to a better understanding of geological processes such as diagenesis, reservoir stimulation, and carbon sequestration, where fluid-rock interactions are crucial.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:****Invited Lecture / 672**

Evolution of subsurface fluid-rock-microbial systems over geologic timescales

Author: Jennifer McIntosh^{None}

Corresponding Author: jenmc@arizona.edu

Our understanding of how complex subsurface porous and fractured rock, fluid, and microbe systems are coupled and have dynamically evolved over geologic time is limited. Yet, this knowledge is necessary for effective subsurface resource and waste management over millennial timescales. Fundamental questions include: How do changes at the land surface alter fluid flow, fluid-rock reactions, and microbial activity at kilometers depth in the earth's crust? How do these reactions and biological activity alter porosity and permeability distributions? And, what evidence of past microbial activity and associated fluid flow and fluid-rock reactions are recorded in minerals precipitated in pore spaces? This talk will highlight recent work on the distribution of permeability and porosity at global-scales and zoom-in to regional- to pore-scale examples of how subsurface microbe-rock-fluid systems have evolved across the Colorado Plateau in response to changes in geologic and hydrologic forcings (e.g., deep burial of sediment versus recent denudation from downcutting of the Colorado River and influx of fresh water). Implications for these findings on the accumulation versus flushing (and/or biological removal) of Lithium-rich brines, helium, hydrogen, and carbon dioxide from pore spaces will also be discussed.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

Invited Lecture / 674**Anomalous Transport in Porous Environments due to Energy Barriers, Self-Propulsion and Dynamic Confinement****Author:** Daniel Schwartz¹¹ *University of Colorado Boulder***Corresponding Author:** daniel.schwartz@colorado.edu

The dynamic behavior of molecules and nanoparticles in confined environments, such as at interfaces and within porous materials, lead to complex and highly-varied phenomena, where heterogeneity may arise from spatial variation of the material/interface itself, from structural configurations, or through inhomogeneous dynamic behavior. To obtain relevant information about these complex dynamics, we have developed highly multiplexed single-molecule/single-particle tracking methods that acquire large numbers of trajectories in a given experiment, enabling robust statistical analysis of anomalous motion. Recent work in our lab has explored the 3D motion of both Brownian and self-propelled nanoparticles within highly interconnected porous environments (both static and dynamic), leading to insights linking microscopic pore-scale mechanisms to macroscopic transport. Examples to be discussed include the barrier-limited diffusive escape of nanoparticles from porous cavities, the enhanced motion of self-propelled catalytic Janus particles within 3D porous materials and the facilitated Brownian diffusion of nanoparticles within dynamically fluctuating porous environments.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:****Poster / 678****Transport and fractionation of explosive byproduct gases through sorptive geomedia****Author:** Chelsea Neil¹**Co-authors:** Daniel Eldridge ¹; Garrett Euler ¹; Hakim Boukhalfa ¹; Hayden Miller ¹; John Ortiz ; Philip Stauffer ¹; Scott Broome ²; Thom Rahn ¹¹ *Los Alamos National Laboratory*² *Sandia National Laboratory***Corresponding Authors:** stauffer@lanl.gov, hmiller@lanl.gov, danieleldridge@lanl.gov, hakim@lanl.gov, cwnil@lanl.gov, john.p.ortiz.14@gmail.com, ggeuler@lanl.gov, stbroome@sandia.gov, trahn@lanl.gov

Discriminating nuclear weapons testing programs from civilian sources is difficult due to highly variable atmospheric radionuclide backgrounds. We aim to study the transport of byproduct gases produced by subsurface explosions, such as carbon dioxide (CO₂) and hydrogen (H₂), as novel signatures for proliferation monitoring. To demonstrate how ratios of gases produced by explosions can change during transport in geomaterials, we conducted laboratory benchtop experiments on the

transport of these gases through variably saturated zeolitic tuff, which is abundant at site of historic US testing. We observed that zeolitic tuff sorbs substantial quantities of CO₂ while allowing H₂ to transport more easily, leading to changes in the molecular ratios of the two gases along the transport pathway. Gas uptake in the dry zeolite core was 72.3% for CO₂, compared with 53.4% for xenon and 7.6% for H₂. The presence of 20% water saturation disrupted the CO₂ sorption process, though to a lesser extent than observed for noble gases, with a 36.7% drop in xenon sorption compared with a 21.9% drop for CO₂. These results represent the first observations of zeolite sorption impacts on explosive gases leading to changes in gas ratios during transport through geomedias relevant to nuclear proliferation monitoring.

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References:

680

idealCompositionalFoam: An extension to the Darcy-scale compositional solver in OpenFOAM

Author: Ali Papi¹

Co-authors: Amir Jahanbakhsh¹; Gabriel Marcos Magalhães²; M. Mercedes Maroto-Valer¹

¹ *Research Centre for Carbon Solutions (RCCS)*

² *PIEP - Centre for Innovation in Polymer Engineering, University of Minho*

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Compositional modelling of multiphase flow in porous media at Darcy-scale is still in its early development stages in OpenFOAM [1]. One critical application of simulating multiphase flow in porous media is in Carbon Capture and Storage (CCS) where the rock and fluids interactions between CO₂ and the host environment can be modelled to predict storage performance. The existing gap in OpenFOAM prevents this powerful Computational Fluid Dynamics (CFD) tool from wider applications in decarbonisation and energy transition aspects.

There are a number of porous media flow solvers in OpenFOAM; however, these packages do not account for compositional simulation (multiphase multicomponent flow with phase interactions) in porous media at the large (i.e. Darcy) scale, as relevant in CO₂ storage processes. At pore scale, compositional simulation is addressed by GeoChemFoam package [2] which couples OpenFOAM flow transport with PHREEQC species reactive transport. Additionally, a multicomponent formulation is implemented in coupledMatrixFoam [3] at Darcy-scale. However, most Darcy-scale packages follow a Black Oil model that treat phases as separate non-interacting continua, e.g., porousMedia4Foam [4] and porousMultiphaseFoam (PMF) [5]. The most famous module of PMF package is impesFoam that solves for incompressible two-phase fluid flow in porous media using IMPES method. Multiple developments of impesFoam exist, including the compressible solution using upstreamFoam [6], groundwater modeller [7], 3-phase solver [8], adaptive mesh refining model [9], hybrid porous-free flow solver using hybridPorousInterFoam [10] and fractured modeller [11].

In an effort to cover the abovementioned gap, we developed an extension to impesFoam called compositionalIGFoam [1, 12], able to account for CO₂/water interactions in CO₂ storage processes in

aquifers using simplified formulations. In this solver, mass transfer between the phases is handled by Henry's and Raoult's laws by assuming equilibrium at each timestep, and hence, skipping the solution to species transport equations. Here, we further developed compositionalIGFoam by updating this code, where the equilibrium assumption is eased, and the species transport equations are solved at each timestep. In the new extension, called idealCompositionalFoam, a sequential approach is adopted. The process is divided into two stages at each timestep: 1) a fully transport process followed by 2) an equilibration stage where mass transfer between the phases is occurred (water evaporating and CO₂ dissolution). In the CO₂/water binary system, one transport equation is solved for one component (e.g. CO₂) in both gas and liquid phases while the other component is calculated by subtracting that mole fraction from one. During the equilibration, equilibrium values are estimated by flash calculations.

The solver was validated by simulating the injection of CO₂ into a water-saturated core model and comparing the results against CMG-GEM. Great agreement was achieved between the two models with only 0.97% and 0.4% difference for water and CO₂ mole fraction values in liquid and gas phases, respectively. The choice of more accurate parameters (density / viscosity and Henry's constant values) compared to previous extension resulted in even more accurate results. In summary, the idealCompositionalFoam extension brings more opportunities to OpenFOAM users for modelling compositional multiphase flow in porous media and associated applications.

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References:

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MS09 / 683

Percolation without trapping with time dependency: modelling Ostwald ripening

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Co-authors: Martin Blunt¹; Branko Bijeljic²

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Conventional measurements of two-phase flow in porous media often use completely immiscible fluids, or are performed over time-scales of days to weeks. If applied to the study of gas storage and recovery, these measurements do not properly account for Ostwald ripening, significantly over-estimating the amount of trapping and hysteresis. When there is transport of dissolved species in the aqueous phase, local capillary equilibrium is achieved: this may take weeks to months on the centimetre-sized samples on which measurements are performed. However, in most subsurface applications where the two phases reside for many years, equilibrium can be achieved. We demonstrate that in this case, two-phase displacement in porous media needs to be modelled as percolation without trapping. A pore network model is used to quantify how to convert measurements made ignoring Ostwald ripening to correct trapped saturation, capillary pressure and relative permeability to account for this effect. We show that conventional measurements over-estimate the amount of capillary trapping by 20-25%.

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Poster / 684

RepoTREND - A Simulation Tool for Safety Analysis of Final Repository for Radioactive Waste

Author: Tatiana Reiche^{None}

Co-authors: D.-A. Becker ; Th. Lauke ; J.W. Wolf

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RepoTREND (Fig. 1) is a novel simulation tool designed for modeling processes in geological repositories for radioactive waste. It enables the analysis of contaminant release, migration through geological barriers, and radiological impacts on the biosphere. The modular structure of RepoTREND allows for flexible and adaptive modeling of different repository subsystems.

The simulation domain of a typical repository is highly heterogeneous, requiring the consideration of multiple physical and chemical processes. RepoTREND incorporates various models, each defined

by specific equations and variables, to represent these processes accurately. The framework supports dynamic model selection for different regions, enabling an adaptive and extensible simulation approach.

The computational core of RepoTREND is based on a fully implicit finite volume method. Physical models are implemented as modular libraries, ensuring transparency and ease of extension. The coupling of models is handled implicitly by solving all equations within a unified matrix system, facilitating seamless integration of new effects while maintaining high computational efficiency.

RepoTREND's advanced capabilities support probabilistic analyses, allowing for comprehensive uncertainty assessments over timescales of up to one million years. These features make RepoTREND a powerful and reliable tool for regulatory safety evaluations and repository performance assessments.

Current Work:

- Near field Module NaTREND: Investigating two-phase radionuclide transport in porous media.
- Repository-Specific Modeling: Implementing rock convergence, compaction processes, and corrosion of metals and cement.
- Thermal Impact Studies: Evaluating the influence of heat-generating radioactive waste on repository stability.
- Computational Optimization: Enhancing numerical methods for improved simulation efficiency and scalability.

References:

- 1 Reiche, T. et al.: Simulation von Nahfeldprozessen in einem Endlager für radioaktive Abfälle, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, GRS-742, Braunschweig, 2025
- 2 <https://www.grs.de/en/news/projects/repotrend-repository-safety-analysis>

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685

Gas Compressibility Effect on Stabilizing Deformation of Wet Granular Media in Hele-Shaw Cells

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Co-authors: Chung Yee Kwok¹; Kang Duan²

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Gas invasion into liquid-filled granular media from a confined geometry is a prevalent phenomenon in geological and environmental applications such as underground carbon storage and oil recovery. This gas-liquid displacement represents one of the most fundamental and common scenarios of two-phase flows. In addition to the typically negligible viscosities, gases are also much more compressible than liquids; as a consequence, the volumetric gas compression will lead to fluctuations

on actual flow rates, thereby exerting a substantial influence on displacement processes and pattern formation. Despite this, previous experimental and theoretical studies have usually simplified both fluids as incompressible, leaving the role of compressibility underexplored. Moreover, the localized fluid-fluid displacement within the granular skeleton frequently mobilizes the host grains, resulting in diverse morphological deformation. Here, we experimentally investigate the effects of gas compressibility on the air-induced deformation of oil-saturated granular media confined in a Hele-Shaw cell. Specifically, we inject air into a monolayer of non-stationary glass beads that are saturated with silicone oil, maintaining a constant nominal flow rate while varying the initial air syringe volumes. We discover that greater compressibility, achieved with larger syringes, has a stabilizing effect on the gas-liquid-grain interface, shifting it from unstable dendritic/ramified fingers to more circular, less branched patterns. The reduced severity of the fingering deformation stems from the decreased compressive pressurization in the gas, which counteracts the viscous depressurization in the displaced liquid. Additionally, we observe that the injection pressure exhibits a non-monotonic evolution, with peak values notably delayed under higher compressibility. Our findings highlight the commonly neglected yet critical role of compression in shaping the gas-driven two-phase flow dynamics in granular media.

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686

The effects of cyclic loading on the conductivity properties of deformable microchannels

Author: Mikhail Turbakov¹

Co-authors: Evgenii Kozhevnikov¹; Evgenii Riabokon¹; Liyuan Yu²; Mikhail Guzev¹; Zakhar Ivanov¹

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In recent years, microfluidic devices have garnered significant attention due to their potential applications in various fields such as biomedical, pharmaceutical and geo-energy researches. These devices often incorporate microchannels with specific geometries and properties, which are critical for their functionality. However, the mechanical behavior of these microchannels under cyclic loading remains largely unexplored, particularly with regard to their conductivity properties. This study aims to elucidate the influence of cyclic loading on the conductivity of deformable microchannels, with a focus on pressure drop measurements and the potential for optimizing conductivity through tailored loading conditions.

Microchannels of varying hydraulic diameters and shapes were fabricated using photopolymerizable resins with controlled elastic moduli. The cylindrical specimens were subjected to cyclic loading under confining pressures ranging from 400 to 2000 psi (2.76 to 13.79 MPa) using a high-pressure biaxial cell apparatus. Our experimental setup included high-precision pressure sensors to measure the pressure drops across the microchannels, allowing us to quantify the changes in flow rates and conductivity under different loading conditions.

The results of our study demonstrate that cyclic loading can significantly alter the conductivity properties of deformable microchannels. Specifically, we observed substantial changes in flow rates and pressure drops within the channels, which were directly correlated with the magnitude of the applied cyclic loading. These findings suggest that the mechanical behavior of microchannels under cyclic loading conditions plays a crucial role in determining their overall performance.

Acknowledgements: This research was funded by the RUSSIAN SCIENCE FOUNDATION project no. 23-19-00699, <https://rscf.ru/project/23-19-00699/>

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MS26 / 688

Advanced Subsurface Characterization using Deep Generative Prior and Reduced Order Modeling

Author: Jonghyun Lee¹

Co-authors: Jichao Bao¹; Jiawei Shen¹; Hongkyu Yoon²

¹ *University of Hawaii at Manoa*

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Subsurface applications like geologic carbon storage and geothermal energy recovery require near-real-time, accurate forecasting for safe and optimized operations. In this presentation, we develop and test an improved data assimilation framework that combines deep generative models as priors in the latent space for parameterization with deep learning-based reduced-order models for rapid thermo-hydro-mechanical prediction during subsurface operations. This framework enables accurate approximation of physical system parameters including permeability, porosity, thermal conductivity, and fault fields.

Our approach employs multiple generative models: variational autoencoders (VAEs) for near-Gaussian-type heterogeneous fields, and both generative adversarial networks (GANs) and latent-space based diffusion models (DMs) for fault/fracture fields. The data assimilation process operates in a latent space of significantly reduced dimensionality compared to the physical parameter space (e.g., « 1M DOF), enabling more effective sampling and improved convergence. During history matching with observation data (e.g., bottom hole pressures at injection wells and pressure, saturation, and temperature at monitoring wells), we update the low-dimensional latent variables, which serve as inputs to the generative models. The resulting outputs are then used in fast reduced-order models for multi-phase flow prediction.

We validate our framework using real CO₂ demonstration data from the Illinois Basin Decatur Project (IBDP) site and field-scale stimulation and circulation tests from the Utah FORGE site. The results demonstrate the framework's capabilities in subsurface property estimation, including uncertainty quantification, prediction accuracy, and computational efficiency for future operations.

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

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Effect of microfractures on the seepage in hydrate bearing rocks under cyclic pressure**Author:** Evgenii Kozhevnikov¹**Co-authors:** Mikhail Turbakov¹; Evgenii Riabokon¹; Mikhail Guzev¹; Zakhar Ivanov¹; Liyuan Yu²¹ Perm National Research Polytechnic University² China University of Mining and Technology**Corresponding Authors:** msturbakov@gmail.com, riabokon.evgenii@gmail.com, kozhevnikov_evgenii@mail.ru

Under cyclic pore pressure, predicting changes in permeability is a crucial factor that determines the overall efficiency of the technology of gas hydrates replacement with carbon dioxide. The classical approach to determining permeability under cyclic pore pressure is the power law, where the exponent is the coefficient of sensitivity of permeability to loading. However, the nature of this coefficient remains poorly understood. Some studies have attempted to establish a relationship between the exponent of the power equation and the porosity or permeability of rocks based on statistical dependencies. Nevertheless, these attempts have not provided a comprehensive understanding of the true nature of the law governing permeability changes. This work presents the results of comparative modeling of the deformation of a porous medium with and without microcracks. Numerical modeling of permeability change with constant and nonlinear Young's modulus was performed. Constant Young's modulus is typical for monolithic samples. The presence of microcracks in samples determines significant deformations and nonlinearity of Young's modulus. Comparison of numerical modeling results with experimental results showed a high degree of convergence.

Acknowledgements: This research was funded by the Ministry of science and higher education of the Russian Federation (Project № FSNM-2024-0008)

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MS14 / 690

An Efficient Approach to Probabilistic Groundwater Flow Modeling for Emergency Well Design

Author: Shang-Ying Chen¹

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Global climate change has intensified extreme meteorological conditions, increasing reliance on groundwater resources, which are less vulnerable to surface water variability, in many regions. Accurately quantifying the uncertainty in hydraulic head due to the heterogeneous hydraulic conductivity of aquifers is crucial for optimizing emergency well placement and determining drilling depth, thereby supporting sustainable environmental water supply management and reliable policymaking. However, the practical implementation of uncertainty quantification is often limited by computational cost. In this study, we employ the Cumulative Distribution Function method, which deterministically solves a system of moment equations along with the equation governing the CDF of hydraulic head, eliminating the high computational burden of Monte Carlo simulations. To further enhance computational efficiency, we use the meshless Generalized Finite Difference method to solve these equations, allowing flexible placement and adaptive distribution of nodes. We apply this framework to the Taichung Basin in Taiwan to demonstrate its effectiveness in generating probabilistic groundwater level distributions for emergency wells. The methodology developed in this work is broadly applicable to real-world groundwater management and other environmental hydrological challenges, providing a robust tool for optimizing well site selection and depth determination in regions facing the risks of surface water scarcity.

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Invited Lecture / 692

Gravity currents in heterogeneous media

Authors: Sepideh Majdabadi Farahani¹; Patricio Hernández-Parra²; Vittorio Di Federico¹; J. Jaime Gómez-Hernández²

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Heterogeneity could be called the “beast” of subsurface modeling. We know that it exists, but often we disregard it because of the complexity of properly handling it. After a quick recall of the importance of heterogeneity in subsurface modeling, we analyze the progression of gravity currents in heterogeneous media under different kinds of heterogeneity, more precisely, multiGaussian realizations, sedimentary-like realizations. The analysis focuses on the time evolution of the free surface as a dense liquid enters a reservoir filled with a much lighter liquid. Probability maps of this surface are built, which measure the uncertainty on the current evolution, and they are compared with the evolution of the same current with a homogeneous conductivity equal to the geometric mean of the heterogeneous realizations.

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Poster / 693

Benchmark for Investigating Coupled Hydro-Geochemical Processes with Gas Production

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Coupled mineral dissolution and precipitation processes with gas production are critical processes in energy subsurface systems, e.g., generating hydrogen gas during the anoxic corrosion of metallic nuclear waste canisters, during natural hydrogen degassing from serpentinized mafic rocks, and CO₂ sequestration in deep saline aquifers. However, the fate of exsolved gas within porous media remains poorly understood. The optimization of these systems relies on understanding underlying hydro-geochemical processes and a realistic system evolution description. Recent advances in multi-phase reactive transport models can predict the long-term behaviour of such systems [1, 2]. However, the challenge remains to describe the coupling between multi-phase flow, the chemical processes, and consequential changes to the transport properties of porous media (e.g., porosity, relative permeability). There is a need to develop experimental benchmarks providing a cross-scale understanding of coupled dissolution and precipitation with gas generation, test and improve implementations of reactive transport models in the description of such phenomena. In this context, we developed a 3D-reactive transport experiment on a macroscopic scale with a simplified chemistry investigating coupled dissolution of BaCO₃, producing CO₂, and precipitation of BaSO₄. The water phase, gas production and transport were imaged by Nuclear Magnetic Resonance Imaging (MRI). SEM analysis revealed a significant pore structure modification through BaSO₄ precipitation in the pore space and on CO₂ bubble surfaces. Especially precipitates on the gas bubbles may influence

transport properties significantly. These experiments provide a robust set of data to benchmark reactive transport models, and we currently concentrate on summarizing our results for setting up such a numerical benchmark.

1 Ahusborde, E., Amaziane, B., de Hoop, S., El Ossmani, M., Flauraud, E., Hamon, F. P., ... & Voskov, D. (2024). A benchmark study on reactive two-phase flow in porous media: Part II-results and discussion. *Computational Geosciences*, 1-18.

2 de Hoop, S., Voskov, D., Ahusborde, E., Amaziane, B., & Kern, M. (2024). A benchmark study on reactive two-phase flow in porous media: Part I-model description. *Computational Geosciences*, 1-15.

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MS09 / 694

Post-breakthrough evolution of viscous fingers

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Viscous fingering instability occurs when a less viscous fluid displaces a more viscous fluid within porous media. It has been extensively studied with pore-scale simulations and bench-scale experiments over the past several decades. Yet the evolution of viscous fingers after the displacement front reaches the outer boundary of the domain is not fully understood (Mora et al., TIPM 2021, Salmo et al., TIPM 2022). Here, we use a combination of microfluidic experiments and pore-network simulations to rationalize the evolution of these patterns under various capillary numbers and viscosity ratios. We discuss our findings in the context of regime crossovers within Lenormand's phase diagram (Lenormand et al., JFM 1988, Primkulov et al., JFM 2021).

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MS06-B / 695

Interference fringe (IF) technique for droplet contact angle and thickness measurement

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Recently, reflection interference fringe (RIF) and transmission fringe techniques (TIF) have been introduced to investigate the origin of far-field interference fringe formation and to determine a droplet's contact angle and thickness. In this study, an integrated analysis of the interference fringe (IF) technique is conducted by varying the schematics, including configuration (transmission/reflection), the droplet's side (left-hand side/right-hand side), and the substrate types (flat/prism). Additionally, the effect of refraction at the droplet edge is considered in relation to the droplet contact angle (sizes), the droplet's refractive index, the zero fringe radius (FR), and the working distance (WD). Moreover, the effects of the maximum incidence angle and the maximum contact angle are investigated. This integrative study demonstrates that a large contact angle range can be measured using a transmission configuration and the droplet's right-hand side. Furthermore, the increasing contact angle trend with the incidence angle on the prism substrate for the droplet's left-hand side is explained through geometric analysis. It is also revealed that the IF technique can determine nanometer-scale thicknesses below 100 nm, corresponding to an ultra-small contact angle of less than 2 micro-radians, with an extended working distance of 3,000 mm. This finding is remarkable, as it shows that nanoscale thickness can be determined using a simple optical configuration under ambient conditions, without requiring a sophisticated setup such as a microscope. It is anticipated that the IF technique can be combined with other nanoscale thickness measurement techniques to enhance its measurement reliability.

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Poster / 696

Measuring Dissolution of Calcium in Natural Limestone via Microscopy and ICP-MS

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Understanding how chemical reactions impact the dissolution rate of rock surfaces over time is critical in subsurface energy activities such as geothermal energy recovery, oil and gas extraction, and carbon storage. Mineral dissolution can increase reservoir permeability as the dissolution can generate permeable pathways, enhancing energy recovery, while other coupled processes such as

weakening of mechanical properties may have an opposite effect. To investigate the effects of chemical reactions on dissolution of a rock surface, experimental studies are conducted using solutions with three different pH levels of 4, 3, and 2 on the surface of an 18 mm x 25 mm polished limestone. This is achieved using a 3D-printed fluidic device that maintains a constant flow rate of 100 $\mu\text{L/hr}$. Effluent is collected about weekly to monitor the calcium concentration (Ca^{2+}) using ICP-MS for assessing the changes of dissolution rate. To gain a clearer understanding of the effects of dissolution along the flow path of the limestone sample, topographic images are captured weekly—one directed towards the inlet and another towards the outlet—at a horizontal resolution of 0.45 μm and a vertical resolution of 0.83 μm using a Zeiss LSM 900 confocal microscope. These images are then compared with the Ca^{2+} concentration to better understand how dissolution occurs both across time and along the length of the flow path. The results indicate that at pH=2, the dissolution is 5x that at pH=3 when measuring Ca^{2+} . Then, within the imaging results, the inlet is shown to have a roughly 2.5x larger dissolution rate than the outlet of the sample for both pH=3 and pH=2. Knowing both the Ca^{2+} concentration and the changes in topography across time, we can further analyze the impacts of pH on dissolution rates over the rock surface roughness and how it may alter surface asperities and change permeability within a reservoir. The next step of this research involves conducting experiments at pH=4 and comparing the results to those obtained at pH=2 and pH=3. Additionally, we will create channels along the limestone surface to investigate how a defined channel affects dissolution across the rock surface. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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697

A Deep Learning-Based Surrogate Model for Pore-Scale Multiphase Flow Field Prediction in Porous Media

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Multiphase flow in porous media is ubiquitous in natural and engineering applications, including carbon sequestration, soil and groundwater engineering, and hydrocarbon recovery. The accurate prediction of pore-scale physical fields is critical for evaluating, optimizing, and controlling the performance of various porous media applications. However, the high-fidelity pore-scale simulation methods are computationally inefficient, requiring hours to days to compute the multiphase flow fields for a single complex case. It is prohibitive when thousands of cases need to be simulated in the application of optimization, parameter study, and inverse modeling. Therefore, an accurate and robust pore-scale surrogate model is imperative to accelerate the porous media flow field prediction.

In this study, a convolutional-based encoder-decoder neural network model was developed to learn the non-linear mappings between porous structures, boundary conditions, and multi-physics fields.

The micro-PIV method was utilized to measure the pore-scale phase and velocity fields, providing high-quality training data for the deep learning model in the supervised learning paradigm. The results show that the proposed deep learning surrogate model can accurately predict the overall patterns of the multi-physics fields for both the single-phase and two-phase porous media fluid flow processes with an accuracy of over 90% on the test datasets. The convolutional-based encoder network effectively learns the high-dimensional features of the porous structures, enabling generalization to various porous structures and scalability to diverse pore sizes. Pertaining to the computational efficiency, the proposed deep learning model can predict the transient two-phase porous media flow fields within 4 milliseconds, which is 4 to 6 orders of magnitude faster than the prevalent high-fidelity pore-scale simulation methods. The deep learning surrogate model developed in this study is computationally efficient and accurate enough to accelerate optimization, parameter study, and inverse modeling for numerous porous media fluid flow applications.

Keywords: Porous media, multiphase flow, deep learning, surrogate model

Acknowledgements: The authors acknowledge funding support from the National Natural Science Foundation of China (No. 52225603).

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MS12 / 699

New insights into unsaturated soil mechanics: analytical derivation of pore-pressure coefficients using a generalized effective stress framework

Author: Angelica Tuttolomondo¹

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Geotechnical operations such as slope excavation, earth dam construction, and drawdown scenarios often involve rapid mechanical loading or unloading in unsaturated soils. These dynamic processes typically progress so quickly that they do not allow for pore water and air migration, thereby inducing significant changes in pore water and air pressures. Accurately predicting these pressure changes is crucial for understanding the mechanical response of the soil. Predicting the induced pore water pressure change for saturated soils involves calculating or experimentally determining the pore-pressure coefficients using effective stress-based analyses. However, similar methodologies for unsaturated soils are lacking. This paper introduces analytical expressions for determining the pore pressure coefficients in unsaturated conditions, employing a generalized effective stress concept. The formulations apply to various stress paths, including isotropic, oedometer, uniaxial, and triaxial,

and they account for the coupled responses of pore water and air pressures under undrained isothermal conditions. The proposed method requires fewer constitutive parameters than existing models; it aligns with traditional formulations for saturated soils at full saturation and uniquely enables the analytical derivation of the undrained soil water retention curve (uSWRC). Traditionally, the SWRC is determined under drained conditions, describing variations in the degree of saturation-suction relationship. In contrast, this study provides the relationship between the degree of saturation and suction during an undrained process, marking a significant departure from conventional practice. The model's performance has been validated against experimental data from diverse loading paths, demonstrating robust correlations in the predicted pore-pressure evolutions. Detailed flowcharts and the "UnDra" computational tool to support engineering applications are provided. This model is particularly valuable for analyzing undrained unloading and loading in overconsolidated states, thus enhancing safety assessments and decision-making for short- and long-term scenarios.

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MS17 / 702

Ion Pairing of Ca^{2+} , Zn^{2+} , and La^{3+} with Acetate is Enhanced in Nanopores

Authors: Bidemi Fashina¹; Anthony Baldo¹; Heath Watts²; Kevin Leung¹; James Kubicki²; Anastasia Ilgen¹

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Nanoscale confined systems are common in the environment and in many technological innovations. Recent studies have shown that the fundamental properties and reactivity of bulk water or unconfined surfaces change under nanoscale confinement. These confinement-imposed changes, in turn, influence several nanoscale processes. Understanding nanoscale processes within confined systems is important for predicting the fate and transport of chemical species, water treatment by nano-filtration, and the fixation of contaminants in porous materials. In this study, we investigated the impact of nanoscale confinement on the ion pairing involving Ca^{2+} , Zn^{2+} , and La^{3+} with CH_3COO^- anions. By modeling the Raman spectra of bulk and confined solutions, we quantified the complexed and uncomplexed acetate species in aqueous solutions and then in the same solutions confined within mesoporous silica with 4 nm cylindrical pores. From these values, we estimated the binding constants and standard Gibbs free energy of ion formation in solution versus in nanopores. The equilibrium constants increased by 0.09, 1.70, and 2.5 units for Ca^{2+} , Zn^{2+} , and La^{3+} – CH_3COO^- , respectively, when compared to analogous constants measured for bulk solutions. Hence, ion pair formation is more favorable in nanopores than in bulk aqueous solutions. Through density functional theory (DFT) calculations, we predicted the stabilization of ion pairs in confined and aqueous environments. In agreement with the experimental findings, the DFT-calculated thermodynamic values for the free energy of formation predict the stabilization of contact ion pairs in confined systems compared to the bulk aqueous environment. These findings have broad implications on the

fate and transport of chemical species in soils and other terrestrial environments and can improve the predictive geochemical modeling of cation-anion complexes in confined systems.

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

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Poster / 703

Development of Deep Learning Based Method for Pore Identification of Core CT Images

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Deep learning (DL) methods are widely used to recognize objects in images. This paper presents a step-by-step workflow to develop a DL-based model for identifying the pores of CT images of core plugs. In this work, some CT images of core plugs are segmented into binary images using threshold method, after post-processing the binary images acting as labels of the original images. The CT images and corresponding labels are fed to a program to generate image-label pairs for building training dataset. A 13-layer semantic segmentation network with 4 convolutional layers is constructed based on deep learning algorithm, and the network is trained with the built training datasets of three different resolutions, respectively. The trained models are tested with different images.

The training results show that the effect of image resolution is obvious and training the network with high-resolution images shows higher accuracy and lower loss. All global accuracy and mean accuracy of different resolution training images are above 0.88. The global accuracy of training network with high-resolution image of low permeability core plug reaches 0.94. The trained network is tested with different images, including images from the same core, images with resolution similar to training images, and low-resolution images. The test results show that the network trained with images whose resolution can capture pores well shows better performance, and the predictive performance of the network trained using low-resolution images is unstable. Compared with the threshold method, the binary image generated by the semantic segmentation method has less noise, thus reducing the post-processing operations of the binary image. Applying the model to batch images with similar grayscale and similar resolution is more efficient than threshold method.

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704

Characterizing CO₂-brine multiphase flow properties of heterogeneous and microporous carbonate rocks with multi-scale eXtensive Pore Modelling (XPM) assisted by machine learning and inversion model

Authors: Zhenkai Bo¹; Hannah P. Menke¹; Julien Maes¹; Ahmed H. Elsheikh¹; Kamaljit Singh¹

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The wide range of pore sizes in carbonate rocks, spanning several orders of magnitude, poses significant challenges for their characterisation using conventional imaging techniques. For example, microporosity, containing nanoscale pores, often remains unresolved in micro-CT scans. Multiscale image-based approaches can be used to address this challenge by segmenting microporous regions in low-resolution images into distinct phases and incorporating high-resolution scans of smaller sub-samples to accurately represent their pore structures. However, understanding the suitability of this method remains a key challenge in effectively modelling the multiphase flow in heterogeneous carbonate rocks. In this study, we present a multiscale characterization and flow modelling strategy for highly heterogeneous carbonate rocks from a formation in Malaysia. Low- (26.4 µm) and high-resolution (165 nm) micro-CT scans were extracted from several rock samples to validate the experimental CO₂-brine relative permeability measurements using multi-scale eXtensive Pore Modelling simulator XPM (<https://github.com/dp-69/xpm>). We found significant contrast between µm-scale and nm-scale simulation results, illustrating the heterogeneity of the rock samples. To integrate different scales, we feed a dense neural network (DNN) model into the ensemble smoother with multiple data assimilation (ESMDA) algorithm to develop the DNN-ESMDA framework. This approach significantly reduces inference time compared to using XPM simulation, allowing us to quantify uncertainty in microporosity phase multiphase flow properties derived from experimental measurements. For validation, we input the inferred microporosity phase relative permeability curves back to XPM and the simulation-based results match well with experimental measurements. Our DNN-ESMDA framework herein provides a critical tool for validating experimental measurements and building digital model for multi-scale porous materials characterization.

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705

Evaluation of acid treatment job for volcanic reservoir with low-resolution images

Author: Hirok Iwama^{None}

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The main objective of the study is to evaluate the potential for using Digital Rock Physics (DRP) technology in the acid treatment study for development of natural gas reservoir. The tasks planned for the study included the creation of three-dimensional models of the pore structures within plug core samples before and after acid treatment using X-ray micro-CT images. This was followed by an evaluation of changes in fluid flow behavior and physical properties within the pores before and after acid treatment. Furthermore, these models were tested under surrounding pressure conditions to simulate pore structure and assess fluid flow behavior and acid flow paths under these conditions.

In this study, volcanic rock samples in the field were used for the experiment. Firstly, image processing was performed to remove noise and clarify the fracture and rock sections using a morphological filter with specified settings. The segmentation of the rock section was performed based on gray value histograms, and the segments included pores, transition areas, rocks, and other regions. Adjustments to segmentation before and after acid treatment showed little difference in the image quality and histogram peaks, indicating minimal impact of acid treatment. The creation of three-dimensional models before and after acid treatment for the samples showed the pore structure and allowed for fluid flow evaluation, despite coarse image resolution compared to the pore structure. Threshold values for differentiation between pores and rocks were adjusted to define flow paths within the sample.

Secondary, estimation of rock properties was conducted introducing some assumptions. One of the challenges for the task was how to deal with voxels which cannot be differentiated between rock and pore, due to coarse resolution of the images. To solve this, specific values such as permeability were defined in those voxels and tuned as matching parameters compared to the actual measurement data in the whole sample.

Finally, flow simulations were conducted to evaluate the change in rock properties after acid treatment. Fluid flow and permeability evaluations for the samples showed significant changes, especially in the core front where pressure and fluid paths adjusted notably. It was confirmed that acid treatment significantly enhanced core permeability, corroborated by fluid flow behavior and pressure changes.

The study summarized the ability to visualize pre- and post-acid treatment fluid behavior in three dimensions and understand acid treatment's impact on flow path shapes. In addition to that, it revealed that a reliable permeability calculation required setting appropriate permeability values for certain voxel segments. Adjustment of segments before and after acid treatment indicated changes in permeability.

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Poster / 706

Directionality of Thermal Diffusive Transport in Subsurface Carbon Dioxide and Hydrogen Storage

Author: Anna Herring¹

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Underground storage of hydrogen (H₂) fuel and carbon dioxide (CO₂) are technologies pursued to mitigate climate change and advance the energy transition. Once injected underground, CO₂ and H₂ will exist as partially-soluble multiphase fluid-water-rock systems: the injected fluids can flow through the porous rock in a connected plume, become disconnected and trapped as ganglia surrounded by groundwater within the storage rock pore space, and also dissolve and migrate through the aqueous phase. Recent analyses —many pioneered by the Benson research team [1,2,3] —have highlighted that the concentration gradients induced by differing capillary pressure between fluid ganglia can drive diffusive transport (“Ostwald ripening”). We build on these previous studies by incorporating the nonideality of gases under geologic conditions, with specific focus on the entropic and thermodiffusive effects resulting from geothermal gradients. Our analysis, based on thermodynamic first principles, provides numerical estimates for CO₂ and H₂ at conditions relevant to underground storage reservoirs. We show that the direction of diffusive transport in isothermal systems is upwards (as found by prior work) for both gases. However, the entropic contributions to the chemical potential of the dissolved species are so significant that we predict a reversal in the direction of diffusive transport —downwards —in deeper storage reservoirs and those with larger geothermal gradients. For CO₂, relatively low geothermal gradients of 10 C/km are sufficient to induce downwards diffusion at depths relevant to storage. Diffusive transport of H₂ is less affected but still reverses direction under typical gradients, e.g., 30 C/km, at a depth of 1000 m. Contrary to previous studies, we find that diffusion and density-driven convection will likely work in concert to drive aqueous phase transport of these fluids: both mechanisms work to drive CO₂ downwards, and H₂ upwards, for conditions representative of their respective engineered storage reservoirs.[4]

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The geological structure of unconventional oil reservoirs is complex, containing a large number of micro-nano pore structures, which makes the exploitation more difficult. The gas injection flooding technology has high application value in the development of unconventional oil reservoirs. CO₂ flooding, N₂ flooding, and foam flooding are all important components of the gas flooding technology, and there are currently many field applications. However, the microscopic mechanism of the oil displacement process, especially the flow process in porous media considering the changes at the oil-gas interface, is still unclear. Accordingly, this study is based on the geometric structure model of real porous media. Using the level set method, the oil displacement processes of CO₂ immiscible flooding, CO₂ miscible flooding, N₂ flooding, and foam flooding are simulated at the microscopic scale. The oil-gas interface is tracked, and the oil displacement laws of different gases are compared and analyzed. Firstly, the dynamic simulation of the gas flooding process is carried out, and the changes of velocity, pressure, and the volume fraction of remaining oil over time are analyzed. Secondly, the influences of factors such as the injection rate, the gas-liquid ratio of the foam, and the surface tension on the oil displacement effect are explored. Finally, under the same conditions, the displacement effects of CO₂ immiscible flooding, CO₂ miscible flooding, N₂ flooding, and foam flooding are compared. By comparing their velocities, pressures, and the volume fractions of remaining oil, the oil displacement processes of different gases under certain conditions are investigated. The research results show that the volume fraction of remaining oil in N₂ flooding and CO₂ immiscible flooding is approximately around 30%. Increasing the injection rates of N₂ and CO₂ can achieve better early-stage oil displacement effects. However, reducing the N₂ injection rate or increasing the CO₂ injection rate can slightly increase the oil recovery rate. The volume fraction of remaining oil in CO₂ miscible flooding and foam flooding is approximately around 5%. Increasing the injection rate of the mixed phase can achieve better early-stage oil displacement effects and slightly increase the oil recovery rate. When the gas-liquid ratio of the foam is 3:1 and the surface tension is 0.02, the volume fraction of remaining oil is the smallest, and the foam flooding effect is the best. The analysis of the oil displacement processes of different gases under the same conditions shows that the inlet pressure in N₂ flooding and CO₂ immiscible flooding drops rapidly, and the final pressure is relatively low. The inlet pressure in CO₂ miscible flooding and foam flooding drops slowly, and a certain pressure is still maintained at the end. Under the micro-scale porous media model, the qualitative analysis shows that the oil displacement effects of CO₂ miscible flooding and foam flooding are better, approximately 95%. The oil displacement effects of N₂ flooding and CO₂ immiscible flooding are relatively weaker, approximately 70%. The research results of this paper have important guiding significance and can provide theoretical support for the effective application of the gas flooding technology.

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708

Simulation of Feldspar Dissolution in Sedimentary Rocks: Integrating Digital Core and Chemical Reaction Kinetics

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Feldspar dissolution is a critical diagenetic process governing the evolution of porous media in sedimentary rocks. However, the differential dissolution mechanisms under open systems (with continuous fluid replenishment) versus closed systems (local chemical equilibrium) remain quantitatively unresolved. This study establishes a multi-process model integrating digital core reconstruction and reaction kinetics to unravel pore-scale dissolution dynamics and their controls on fluid storage capacity in sedimentary systems. Leveraging 2D mineralogical maps from AMICS scanning, a machine learning-derived 3D digital core model was developed, achieving high consistency with the 2D mineralogical data. A reaction kinetic model for open/closed systems was formulated using transition state theory and Arrhenius rate equations. Simulations demonstrate that open systems drive a pore-enhancement phase with permeability increase, while closed systems promote secondary mineral precipitation and permeability reduction during pore reconfiguration. In feldspar-rich siltstone lithofacies, dissolution-generated porosity (>3.5%) dominantly hosts free-phase fluids, with total gas storage exceeding 5.0 m³/t. The integration of digital core and reaction kinetics provides a transformative framework for modeling mineral-fluid interactions across scales, with direct implications for hydrocarbon recovery, CO₂ sequestration, and geothermal energy extraction in sedimentary basins. This work is funded by the National Natural Science Foundation of China (42202146 and 42372156), Taishan Scholars Program (tsqn202408104), Fundamental Research Funds for the Central Universities (24CX06015A and 24CX02001A), Natural Science Foundation of Shandong Province (ZR2022QD029), Fund of State Key Laboratory of Deep Oil and Gas, China University of Petroleum (East China) (SKLDOG2024-KFYB-02 and 24CX02001A), and Open Fund of SINOPEC Key Laboratory of Geophysics (36750000-25-FW 0399-0006).

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Poster / 710

Assessment of the Effectiveness of 2.5D Pore-Scale Modeling

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Digital rock physics (DRP) is an emerging technique that integrates advanced imaging and computational modeling to characterize rock microstructures. The flow transport properties such as absolute permeability, velocity, and relative permeability can be quantified using numerical simulations based on high-resolution three-dimensional (3D) digital rock models. However, the acquisition and simulation of 3D models are often expensive and computationally demanding. Two-dimensional (2D)

models are more accessible alternatives and are frequently utilized in microfluidic experiments but those models commonly fall short in capturing pore-scale trapping phenomena or relative permeability curves. As another alternative, 2.5D models^[1] have been introduced to bridge the gap. In 2.5D models, the etching depth of each void (pore) pixel in a 2D image depends on its distance from the nearest solid (grain) pixel, enhancing the geometric representation of pore throats. The etching depth or shape were still limited because they were devised for micromodel experiments. In this study, we generated digital 2D and 2.5D models for a range of parameters including the slice number of a 3D rock image, etching depth, and etching shape. We compared their transport properties such as relative permeability versus saturation, as well as quantifying the topology of the trapped non-wetting phase, to those of the original 3D model using the open-source Lattice-Boltzmann simulator OPM/LBPM. The quantitative and qualitative results demonstrate the capabilities of 2D and 2.5D models to replicate essential transport properties of 3D porous media they represent.

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^[1] Xu, K., Liang, T., Zhu, P., Qi, P., Lu, J., Huh, C., & Balhoff, M. (2017). A 2.5-D glass micromodel for investigation of multi-phase flow in porous media. *Lab on a Chip*, 17(4), 640–646. <https://doi.org/10.1039/C6LC01476C>

711

A 3D mathematical model of column adsorption and comparison to averaged 1D models

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Fluid flow and mass transport in porous media involving mass transfer between the fluid phase and the solid matrix occurs in a great variety of applications. One such application is capturing a contaminant from a carrier fluid forced through an adsorbing column. Describing this process in realistic 3D porous geometries is complex. A standard approach involves reducing the governing equations describing the process to one spatial dimension via averaging procedures [1,2]. These models can be solved analytically in some limiting cases. The obtained solutions can be implemented in optimisation routines to find unknown parameters of the process such as the adsorption rate [3]. However, the details of the 3D microstructure are difficult (or impossible) to capture in 1D models and they are often lost in the averaging procedure. This makes it difficult to analyse the possible effects of the microstructure in the adsorption process. In this talk, we will formulate and solve a 3D mathematical model of contaminant capture by adsorption in 3D idealised porous media. The results of the simulations will be compared with the solutions of averaged 1D models [4]. We will show how the solution of the 1D models is very accurate for typical experimental operating conditions.

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Student Awards:**Water & Porous Media Focused Abstracts:****References:**

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Poster / 712

Evolution of Capillary Trapping of scCO₂ Under Repeated Drainage-Imbibition (D-I) Cycles on Bentheimer Sandstone.

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Keywords: Drainage, Imbibition, Capillary trapping, Residual Saturation

Capillary trapping of supercritical CO₂ (scCO₂) in porous media is a key mechanism that enhances the security of geologic carbon storage. However, the pore-scale processes that control trapping efficiency, especially under repeated drainage-imbibition (D-I) cycles, are not yet fully understood. In this study, we performed a series of core-scale experiments designed to quantify the evolution of capillary trapping behavior in Bentheimer sandstone. Three cycles of drainage and imbibition were conducted using scCO₂ and deionized water, under reservoir-relevant temperature and pressure conditions of 40°C and 1250 psi respectively on a Bentheimer Sandstone of 6 inches length, 1.5 inches diameter and 20% estimated porosity. Pressure differential across the core was continuously monitored during each cycle to capture dynamic fluid displacement events. Distinct pressure signatures were observed: drainage events were characterized by sharper rises or spikes in differential pressures due to capillary resistance of scCO₂ invasion into water-occupied pores, while imbibition phases showed lower rises in differential pressure aided by the water-wetting nature of the Bentheimer sandstone. The capillary numbers for drainage and imbibition were calculated as 6.37E-7 and 5.7E-7 respectively, indicating capillary-dominated flow in both phases.

Injection during both drainage-imbibition phases was continuous, without flow interruptions and core-averaged saturation was calculated based on a mass balance of fluids, recorded via acoustically-monitored separator during injection. These saturation measurements quantify the residually trapped scCO₂ saturations after each drainage-imbibition cycle, providing a direct metric for trapping efficiency. Preliminary results indicate that repeated imbibition cycles lead to progressive increases in trapped scCO₂ volumes, consistent with enhanced capillary trapping due to pore-scale hysteresis

effects. Observed trends in pressure and saturation are being analyzed to better understand the relationship between pore throat distribution, wettability evolution, and trapping performance. This experimental work serves as a foundational component of broader research aimed at linking pore-scale mechanisms to core- and reservoir-scale trapping behavior. Ongoing efforts include high-resolution micro-CT imaging of selected core samples and numerical pore-network modeling to simulate multiphase flow and validate experimental findings. By integrating experimental observations with imaging and modeling approaches, we aim to provide a comprehensive understanding of capillary trapping controls across scales. The findings will contribute to better predictions of CO₂ retention in geologic formations and improve storage design and evaluation.

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713

Multiscale modeling of adsorption in porous media, from surface interactions to effective 1D transport

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In this talk, we present recent advances in the mathematical modeling of adsorption processes, widely employed to remove contaminants from liquids and gases. Traditionally, this field has relied on experimental and numerical methods, typically limited to laboratory-scale settings where the adsorbent microstructure is averaged out.

We introduce a novel 3D mathematical model that accurately describes contaminant adsorption in columns with arbitrary porous configurations. The model consists of a system of partial differential equations: an evolution equation on the surface of the porous medium captures mass transfer by adsorption, while Stokes flow and an advection-diffusion equation govern contaminant transport through the interstitial fluid. Assuming a finely structured porous medium formed by a periodic array of grains, we apply homogenization theory to rigorously derive an effective 1D model. While maintaining the same mathematical form as the classical 1D column adsorption equation, the up-scaled model introduces a dispersion coefficient that explicitly reflects the microstructural properties of the porous medium.

This approach offers a rigorous theoretical foundation for the standard 1D model and provides a framework for analyzing adsorption columns with heterogeneous pore size distributions. Furthermore, it can be readily extended to incorporate detailed physico-chemical surface interactions.

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714

Microfluidic model of micro-haemodynamics in porous media**Authors:** Qi Chen¹; Eleanor Doman¹; Oliver Jensen¹; Igor Chernyavsky¹; Anne Juel¹¹ *University of Manchester***Corresponding Authors:** anne.juel@manchester.ac.uk, qi.chen-27@postgrad.manchester.ac.uk, eleanor.doman@manchester.ac.uk, oliver.jensen@manchester.ac.uk, igor.chernyavsky@manchester.ac.uk

The human placenta is a crucial life support system for the developing fetus, which relies on well-orchestrated haemodynamics to deliver its multiple functions [1]. However, quantifying the flow of red blood cells (RBCs) within the placental porous intervillous space (IVS), where the particulate nature of RBC suspension cannot be ignored, remains an open problem. We address this knowledge gap by employing a novel experimental biomimetic approach based on a suspension of ultra-soft deflated polydimethylsiloxane (PDMS) microcapsules, which are capable of large deformations and reproduce typical dynamics of RBC in steady flow [2].

We fabricate large numbers (tens of thousands) of such tuneable PDMS microcapsules to investigate soft suspension flows in both ordered and disordered planar porous media, informed by 3D imaging of placental tissue [3]. Our model indicates a scaling relationship for the excess resistance as a function of the elasto-viscous capillary number of the capsule and the suspension volume fraction. This rheological relationship demonstrates a surprising invariance to microstructural variations in the porous media.

We further demonstrate that the capsule suspension flow in a disordered porous medium can amplify heterogeneity via preferential pathways and clogging mechanisms. Finally, we show how the interaction of suspension flow with the geometry of a porous medium results in anomalous lateral dispersion dynamics of individual capsules, which could have implications for tissue oxygenation.

This study could also contribute to a better understanding of micro-haemodynamics and haematopathology in other complex microvascular tissues.

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716

Solid-Gas reaction modeling using the Shrinking Core framework

Author: Cristian Moreno-Pulido¹

Co-authors: Francesc Font²; Tim Myers³; Rachael Olwande⁴

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The shrinking core model (SCM) is a widely employed mathematical framework for the analysis of heterogeneous reactions, with applications in hydrogen storage technologies, pharmacology, and various chemical engineering processes. Traditional SCM approaches often assume a single rate-controlling step, which limits their applicability in describing experiments. In this work, we extend the classical SCM by incorporating both numerical and semi-analytical techniques, enabling the treatment of processes governed by multiple interacting mechanisms. Our generalized approach captures more realistic dynamics and provides a rigorous mathematical formulation, offering improved modeling accuracy for industrial processes.

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717

Early Diagenesis as an Analogue for CO₂ Mineral Trapping: A Quantitative Comparison of Fluid-Rock Interactions Using 1D PHREEQC Reaction Path Modeling

Authors: Venkateshwaran Baskaran¹; AKM Eahsanul Haque¹; Numair Ahmed Siddiqui¹; Hariharan Ramachandran²; Ramkumar Muthuvairavasamy³

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Geological carbon sequestration (GCS) represents a promising approach for mitigating carbon emissions, yet predicting long-term mineral trapping mechanisms remains challenging due to the extensive timescales involved. Natural CO₂ fields observations, numerical simulations, and laboratory

experiments can be helpful to attain the mineralization processes. This study investigates early diagenetic processes in deep marine turbidites from the Bengal Fan (ODP Leg 116, Hole 717C) as natural analogues for understanding in-situ CO₂ mineral trapping. We employed 1D PHREEQC reactive path modeling to quantify mineral saturation indices across different biogeochemical zones and compared these with observations from established natural CO₂ reservoirs.

Our analyses reveal distinct mineral stability relationships between the sulfate reduction zone (maximum depth ~400m) and the deeper methane fermentation zone (extending to ~1500m) (Figure-1a). The deep methane fermentation zone (856m) shows significant improvements in iron mineral saturation states following simulated CO₂ injection, with siderite and hematite saturation indices increasing by +8.97 and +16.34 respectively, while K-mica experiences only modest negative shifts (SI change: -1.95) (Figure-1b). We observed consistent equilibrium states for dawsonite (SI: 0) across all depths after CO₂ injection, suggesting thermodynamic potential for formation. However, this likely overestimates actual precipitation rates due to kinetic limitations and restricted aluminum mobility, consistent with field observations from natural CO₂ reservoirs in the Colorado Plateau and Southern Rocky Mountains province, including Bravo Dome (New Mexico), Springerville-St. Johns Dome (Arizona/New Mexico), McCallum Dome, Sheep Mountain, McElmo Dome, and Green River (Utah).

These natural analogues from various geological settings—spanning Permian sandstones to Cretaceous and Jurassic formations—provide critical insights into long-term trapping mechanisms. Additional comparisons with North Sea Fields (Fizzy Field in Permian Rotliegend Group), Ladbroke Grove Field (Australia), and active injection sites such as the Otway Basin and In Salah CO₂ storage project at Krechba, Algeria, demonstrate that mineral saturation states observed in natural systems often differ from theoretical predictions. These comparisons highlight the limitations of equilibrium-based models in representing the temporal dynamics of mineral trapping processes. Natural CO₂ fields may therefore be regarded as being at a more advanced stage of reaction than the laboratory experiments.

Our findings demonstrate that biogeochemical zonation in early diagenetic batch reactor regions provides valuable insights into complex reaction pathways involving redox processes, microbial activities, and mineral transformations relevant to anthropogenic CO₂ storage. Further investigation across different depositional environments beyond deep marine turbidites, including deltaic, shelf, reef, and fluvial settings, is necessary to comprehensively validate early diagenesis as an analogue for CO₂ mineral trapping. This approach integrates natural process observations with experimental data to enhance predictive models for long-term carbon sequestration security and effectiveness.

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Poster / 718

Intercalation of TCE and PFAS Into Interlayer Spaces of Montmorillonite Clay and Sediment-Associated Clay Minerals

Author: Donald Matthieu¹

Co-authors: Jacqueline Maximillian ²; Joan Curry ²

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TCE (trichloroethylene), PFAS, and other chlorinated solvents are common contaminants at hazardous waste sites, both in the United States and globally. These compounds pose significant risks to human health due to their toxicity and persistence in the environment. TCE enters the subsurface from industrial operations such as aircraft cleaning, metal degreasing, and improper disposal of industrial waste. PFAS is introduced into the subsurface from fire training and firefighting operations as well as fluorochemical manufacturing facilities.

Field investigations at multiple hazardous waste sites have shown that higher concentrations of PCE (tetrachloroethylene) and TCE can exist in clay lenses in contamination source zones or contaminant plume areas at hazardous waste sites. At a hazardous waste site in Arizona, plume remediation efforts caused a significant difference in the mass removal between a gravel unit and a clay unit and this suggests that the clay unit at this site is serving as a long-term back diffusion source of TCE. The clay layers at such sites often contain montmorillonite, a smectite clay mineral that intercalates molecules into the interlayer spaces present in these minerals. These interlayer spaces typically intercalate exchangeable cations such as calcium, sodium, and magnesium, but studies have shown that TCE can also intercalate into these interlayer spaces in conditions where this contaminant is present in the subsurface. At a hazardous waste site in Arizona, the intercalation of TCE has been found to occur in field clay samples. TCE intercalation was also found to occur with specimen clay samples that were evaluated in the same study. In addition to TCE, multiple other types of organic contaminants have been shown to intercalate into clay interlayer spaces. It has also been suggested that TCE intercalated into interlayer spaces may contribute to extensive elution tailing observed in column experiments examining TCE mass removal.

Recent research in this area has included more experiments to examine intercalation of TCE into interlayer spaces of clays, in combination with other contaminants that exist at hazardous waste sites. Mixtures of TCE waste, PCE waste, and surfactants have been studied to determine if these compounds intercalate into the montmorillonite interlayer spaces. At a hazardous waste site in Arizona, PFAS contamination exists with TCE contamination. While PFAS intercalation into interlayer spaces of clays has been studied, no research to date has investigated intercalation behavior when clays are exposed to a combination of contaminants that include TCE and PFAS. Future research will include measuring changes in montmorillonite interlayer spacing in clays exposed to a mixture of aqueous TCE and PFAS using specimen clays and field samples. These experimental conditions are representative of the field conditions at a hazardous waste site in Arizona.

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719

Approximate solutions to the Shrinking Core Model and its interpretation

Authors: Cristian Moreno Pulido¹; Francesc Font²; Rachael Olwande³; Tim Myers⁴

¹ *Universitat de Girona*² *Universitat Politècnica de Catalunya(UPC)*³ *niversitat Politècnica de Catalunya (UPC)*⁴ *Centre de Recerca Matemàtica(CRM)***Corresponding Authors:** cristian.moreno@udg.edu, tmyers@crm.cat, francesc.font@upc.edu, rachael.olwande@upc.edu

The shrinking core model (SCM) is a standard tool for describing the evolution of a sphere where material diffuses towards a central solid core and reacts at a moving interface. This model has been widely used to represent various fluid-solid reactions in chemical engineering, metallurgy, and environmental processes. In many of these applications, flow transport through a porous medium plays a critical role, such as in hydrogen storage in metal hydrides. Typically, the SCM is reduced under the Pseudo-Steady State (PSS) assumption, which permits the time derivative to be neglected in the diffusion equation and an exact analytical solution is obtained. By applying the PSS simplification, the system of equations becomes more tractable, allowing for a clearer understanding of the dominant physical mechanisms. In this work, we examine the assumptions made in the PSS to ascertain when it holds, how this affects the interpretation of data, and how to progress if the PSS cannot be applied. Particular attention is given to identifying the conditions under which deviations from PSS behavior become significant, and to proposing systematic approaches for dealing with cases where the steady-state assumption breaks down.

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Separating 3d-elements by reactive nanopores within functionalized zirconium-based metal-organic framework

Authors: Boyoung Song¹; R. Eric Sikma²; Melissa L. Wygant¹; Kevin Leung¹; Dorina F. Sava Gallis¹; Anastasia G. Ilgen¹

¹ *Sandia National Labs*² *Miami University***Corresponding Author:** boysong@sandia.gov

Recycling and separating critical minerals (CM) such as manganese (Mn²⁺), cobalt (Co²⁺) and nickel (Ni²⁺) from electronic wastes can help secure the global critical mineral (CM) supply and clean energy production. Metal-organic frameworks (MOFs) are a promising material class to effectively sequester CMs from heterogeneous aqueous solutions due to their large surface areas, large pore volumes and size, and tunable reactivities. Functionalization of MOFs can modify the ion-binding properties of these materials, prompting the metal-specific chemical chelation towards target CMs, enhancing the sequestration capacity. Zirconium-based MOF (MOF-808) was investigated for its selective adsorption behavior in the absence and presence of nitrogen containing functional groups, pyrazole (MOF-808-PyC). Pristine MOF-808 shows an adsorption trend of Mn²⁺ > Co²⁺ ≈ Ni²⁺ while this trend changes for MOF-808-PyC, showing the increased selectivity towards Ni²⁺ followed by Mn²⁺ and Co²⁺. This result suggests i) the sorption mechanisms are different between MOF-808 and MOF-808-PyC which can be metal specific and ii) pyrazole has stronger affinity to Ni²⁺ over Co²⁺

and Mn²⁺. X-ray absorption fine structure spectroscopy (XAFS) indicates that Ni²⁺ has a similar local coordination environment in the pristine MOF-808 and in pyrazole-functionalized MOF-808-PyC. XAFS shows that Ni²⁺ coordinates to the Zr-metal oxo-cluster. Furthermore, X-ray photoelectron spectroscopy indicates that electronic environment around nitrogen changes with Ni²⁺ adsorption, unambiguously indicating that nitrogen-containing groups, such as pyrazole, impact the selectivity of MOF-808. This likely indicates, that there are several types of surface complexation for Ni²⁺ in MOF-808. Our study provides important scientific insights for the design of new materials for ion separations that are relevant for CMs recycling, specifically for cathode recycling from lithium ion batteries.

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed herein do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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Poster / 723

Transformative Effects of Nano-MgO Integration in Electrokinetic Soil Conditioning: A Systematic Analysis of Expansive Clay Stabilization

Author: Najibullah Zulfeqar¹

Co-authors: Ali Khosravi¹; Shiqiang zou¹

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Expansive soils are widely known for their high shrink-swell behavior, which can lead to substantial structural damage and maintenance challenges in civil infrastructure. Traditional stabilization methods often face limitations in achieving uniform treatment and long-term effectiveness. In recent years, nanoparticles have emerged as a promising alternative for soil stabilization due to their high surface area, reactivity, and ability to alter soil fabric at the microstructural level. This study first evaluated the effectiveness of MgO and SiO₂ nanoparticles through physical mixing tests. Among the two, MgO demonstrated superior performance, showing significant improvements in plasticity characteristics, including an increase in the plastic limit, a 22.78% reduction in the plasticity index, and a near elimination of swell potential at a 3% concentration. Based on these results, MgO was selected as the optimal nanoparticle for further enhancement using electrokinetic conditioning. The electrokinetic technique was employed to facilitate uniform distribution of MgO throughout the soil matrix. The integrated electrokinetic-MgO approach yielded substantial improvements, including a 28.26% reduction in swell strain and a 221.39% increase in compressive strength near the cathode at a MgO-to-water ratio of 1:10. X-ray fluorescence confirmed effective MgO distribution throughout the soil matrix.

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Poster / 724

Phase redistribution in heterogeneous porous media during periods of no-flow

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Subsurface gas storage will involve next to periods of injection and production, periods of no-flow. During these no-flow periods, redistribution of the liquid and gas phases can occur, driven by dissolution and exsolution processes. To better understand this redistribution, we have carried out microfluidic drainage and imbibition experiments, using pre-equilibrated CO₂ and water, after which the system was isolated. Experiments were conducted under two configurations: 1. Fully isolated (undrained) system, where the chip was sealed at the inlet and outlet. 2. Connected outlet system, where the chip was sealed at the inlet, but the outlet was connected to a small reservoir filled with CO₂, mimicking a connection to a highly porous rock or fracture. The pH indicator Bromothymol Blue was used to monitor the amount of dissolved gas in the water. In the fully isolated (undrained) system, redistribution was observed due to the dissolution-driven process of Ostwald ripening. In the connected outlet system, gradual gas exsolution occurred over time. The results of these experiments suggest that local pressure variations arising from rock heterogeneity make redistribution during periods of no flow significantly more complex than can be explained by Ostwald ripening alone.

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