France InterPore Chapter

17^{e} Journées d'Etudes des Milieux Poreux

Du 4 au 6 novembre 2025 à Orléans

Domaines variés / *Various topics*

Stockage de l'énergie / *Energy storage*
Géothermie / *Geothermal energy*
Génie civil / *Civil engineering*
Dépollution / *Remediation*
Energies renouvelables / *Renewable energy*
Agroalimentaire / *Food industry*
Santé / *Health*
Matériaux / *Materials*…

Interdisciplinarité / *Interdisciplinarity*

Mathématiques appliquées / *Applied mathematics*
Mécanique des fluides / *Fluid mechanics*
Transferts de chaleur et de masse / *Heat and mass transfer*
Génie des procédés / *Process engineering*
Géosciences / *Geosciences*
Transport réactif / *Reactive transport*
Modélisation numérique / *Numerical modeling*
Microfluidique / *Microfluidics*…

Orateurs invités / Invited keynote speakers:

Lydéric Bocquet, Ecole Normale Supérieure, Paris
Laurent Brochard, Laboratoire Navier, Champs-sur-Marne
Carla De Tomas, Imperial College London (Grande-Bretagne)
Jennifer Druhan, University of Illinois Urbana-Champaign (Etats-Unis)
Rainer Helmig, University of Stuttgart (Allemagne)
Sylvie Lorthois, Institut de Mécanique des Fluides de Toulouse

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Mardi 4 novembre

salle / *room*:		plénière	salle atelier 1	salle atelier 2
08:30	Accueil café / *Coffee*			
08:45	Mots de bienvenue / *Welcoming words*			
09:00	Keynote 1	**Rainer Helmig**, University of Stuttgart (Germany), Kimberly-Clark Distinguished Lecturer 2025 of the International Society for Porous Media		
09:45	Pause café / *Coffee break*			
10:15	Sessions parallèles 1	*Imagerie et caractérisation des milieux poreux I*	*Transport colloïdal et particulaire en milieu poreux*	*Milieux confinés, nano-échelles et modélisation moléculaire*
11:55	Déjeuner / *Lunch*			
13:45	Keynote 2	**Jennifer Druhan**, University of Illinois Urbana-Champaign, Institut de Physique du Globe de Paris		
14:30	Sessions parallèles 2	*Ecoulements multiphasiques en milieux poreux I*	*Mécanique, poromécanique, rupture, endommagement*	*Mésoporeux*
15:50	Pause café / *Coffee break*			
16:15	Sessions parallèles 3	*Microfluidique*	*Transfert thermique en milieux poreux*	*Transferts en milieux fracturés*
17:35				
18:00	Cocktail de bienvenue / *Welcome reception* - Musée des Beaux-Arts			

Mercredi 5 novembre

salle / *room*:		plénière	salle atelier 1	salle atelier 2
08:30	Accueil café			
08:45	Keynote 3	**Carla de Tomas**, King's College London (UK)		
09:30	Sessions parallèles 4	*Imagerie et caractérisation des milieux poreux II*	*Transport réactif I*	*Méthodes numériques*
10:30	Pause café / *Coffee break*			
11:00	Sessions parallèles 5	*Imagerie et caractérisation des milieux poreux III*	*Milieux poreux biologiques I*	*Ecoulements multiphasiques en milieux poreux II*
12:20	Déjeuner / *Lunch*			
14:00	Keynote 4	**Lydéric Bocquet**, Ecole Normale Supérieure (Paris)		
14:45	Sponsors	Présentation des sponsors / *Sponsor presentations*		
15:15	Sessions parallèles 6	*Modèles numériques et couplage pour les milieux poreux*	*Transport, mélange et dispersion en milieu poreux*	*Fluides complexes, non-newtoniens, inertiels et turbulents*
16:35	Pause café - posters / Coffee break - posters			
17:30	Assemblée générale / FIC general assembly			
19:00	Dîner de gala / *Gala dinner*			

Jeudi 6 novembre

salle / *room*:		plénière	salle atelier 1	salle atelier 2
08:30	Accueil café			
08:45	Keynote 5	**Sylvie Lorthois**, Institut de Mécanique des Fluides de Toulouse		
09:30	Sessions parallèles 7	*Imagerie et caractérisation des milieux poreux IV*	*Couplages multiphysiques en milieux poreux I*	*Milieux fibreux*
10:30	Pause café - posters / *Coffee break - posters*			
11:30	Sessions parallèles 8	*Transport réactif II*	*Couplages multiphysiques en milieux poreux II*	*Ecoulements multiphasiques en milieux poreux III*
12:30	Déjeuner / *Lunch*			
14:00	Keynote 6	**Laurent Brochard**, Laboratoire Navier, Ecole Nationale des Ponts et Chaussées		
14:45	Sessions parallèles 9	*Transport réactif III*	*Milieux poreux biologiques II*	*Couplages multiphysiques en milieux poreux III*
16:05	Pause café / *Coffee break*			
16:20	Clôture / *Closing words*			
16:30	FIN / *END*			
19:00	Conférence grand public au Mobe			

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Free and bound water transport during drying of a clay material as observed by NMR

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Keywords: Clay paste, Drying, NMR, adsorbed water

Raw earth, an ancestral building material, is experiencing renewed interest thanks to its mechanical and hygrothermal properties, as well as its low environmental impact. It generally contains a significant proportion of clay, which plays an essential role in its overall performance.

In this context, we are interested in kaolin, a clay that is used as a model material for the analysis of raw earth drying mechanisms. Because of its fine, well-characterized mineral structure, kaolin is a relevant basis for studying water transfer mechanisms similar to those observed in materials such as adobe, compacted earth or cob. The aim of our work is to examine the behavior of the material during the entire drying process, from the initial pasty state to the final stages of water extraction at the nanometric scale.

Initially, a paste is prepared by mixing kaolin and water in controlled concentrations. The drying process of this paste is then studied using Nuclear Magnetic Resonance (NMR), a technique for quantifying changes in the characteristics of the transverse relaxation time distribution (integrals under the peaks, peak widths and mean relaxation times) over time. At the same time, Magnetic Resonance Imaging (MRI) enables us to visualize the spatial distribution of water within the sample. To assess the influence of environmental conditions on the process, different dry air flows, applied at varying speeds, were applied to modulate drying.

The process takes place in several stages: first, a homogeneous contraction of the paste is observed, resulting in a reduction of porosity and pore size, while the drying rate remains constant. During this phase, due to capillary action, the residual water is redistributed within the paste toward the evaporation zone located at the interface with the air, allowing contraction to continue until the solid structure stabilizes and further rearrangement is no longer possible. Subsequently, the material becomes rigid but continues to gradually desaturate: this is the phase during which the drying rate decreases.Particular attention is then paid to the final stage, i.e., the diffusion of adsorbed water, initially present in the form of films approximately ten molecular layers thick, and to the resulting dynamics of transfer through the porous matrix.

Experimental Study of Tidal Oscillatory Flows on a Partially Saturated 1D Porous Column

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Keywords: Oscillatory flows, Tide machine, Partially saturated media, Unsaturated porous media, Darcy-scale experiments, Soil parameter estimation, Frequency response.

This article aims at investigating experimentally the impact of low-frequency waves (such as tides) on the behavior of a partially saturated vertical porous column in a sand beach. The study involves applying an oscillatory pressure, represented by a simple harmonic function, at the base of the sand column.

A detailed description of the experimental setup is provided, including the Darcy-scale soil column apparatus, and the hydro-mechanical system (referred to as the "tide machine") used to simulate the tidal forces. We outline the methods employed to calibrate the measurement sensors, particularly the tensiometers used to measure both positive and negative pressures with respect to atmospheric pressures, at various elevations along the sand column.

Some results and interpretations are presented based on the available range of forcing parameters. These results include analyses of pore water pressure signals, total pressure signals, and water table elevation, along with the corresponding pressure profiles and total head profiles. Key findings, such as signal attenuation, phase lag, and non-harmonic behavior, are thoroughly discussed.

Additionally, the article illustrates the estimation method used in the physical experiments to obtain the hydrodynamic unsaturated parameters of the sand (hydraulic conductivity and water retention curves). This is achieved through an inverse problem-solving approach that employs a Genetic Algorithm (GA). The calibrated sand parameters are intended to support future numerical simulations of the experimental results including for example fixed-grid Finite Volume, or Lagrangian methods like the Moving Multi-Front method.

References

Ababou, R., Alastal, K., Astruc, D., Al-Bitar, A., Marcoux, M., & Wang, Y., Model coupling for environmental flows, with applications in hydrology and coastal hydrodynamics, La Houille Blanche, 101(2), 9–24 (2015) https://doi.org/10.1051/lhb/20150014

Alastal, K., & Ababou, R, Moving Multi-Front (MMF): A generalized Green-Ampt approach for vertical unsaturated flows, Journal of Hydrology, 579, 124184 (2019). https://doi.org/10.1016/j.jhydrol.2019.124184

Alastal, K., Ababou, R., Astruc, D., & Mansouri, N, One-dimensional oscillatory flows in partially saturated media with moving multi-front, Physics of Fluids, 37(2), 026626 (2025). https://doi.org/10.1063/5.0251587

An Efficient Approach to Fluid Flow and Heat Transfer in Fractured Porous Media: Applications in Geothermal Energy

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Keywords: Geothermal energy, fractured porous media, discrete fracture matrix model, heat transfer

Abstract

Geothermal energy has gained increasing attention as a sustainable energy source in the recent years. A significant portion of geothermal processes occurs in highly fractured rocks where complex structures necessitate advanced modelling techniques to accurately simulate fluid flow and heat transport. For this purpose, several modelling approaches have been developed, and these can be broadly classified into two categories:(a) Implicit approaches which are based on upscaling the properties of the medium, offering computational efficiency but sacrificing accuracy in capturing localized fracture-matrix dynamics; (b) Explicit approaches (e.g., Discrete Fracture Matrix models (DFM)), where the fractures are explicitly represented. While DFM models provide accurate solutions, the computational cost increases significantly, especially in densely fractured reservoirs without any simplifying assumptions.

In this study, we investigate various modelling approaches for enhancing computational efficiency without significant loss of accuracy depending on the flow conditions. First, we derive a coupled DFM which captures both convection and conduction in the fractures while assuming only conduction in the matrix (i.e. neglecting the flow due to low permeability). The model is developed within a hybrid-dimensional framework, where the matrix is represented as n-dimensional elements and the fractures as (n-1)-dimensional elements (for this study n is taken equal to 2). The resulting system of partial differential equations is discretized with the finite volume method and solved using advanced numerical solvers. The model has been validated against numerical simulations carried out with the commercial software COMSOL Multiphysics. In a second step, we test our capability of deriving upscaled models that simplify the matrix and/or fracture representation. The objective for such development is to further increase the computational efficiency when we have a highly fractured rock. An embedded fracture modeling approach will be investigated as a first attempt to explore such feasibility. Sensitivity analyses will be performed to present the domain of application and the range of validity of this formulation.

Gas adsorption characterization of biochar: surface area, pore size distribution, and sorption energy

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Keywords: Biochar, Gas adsorption, Surface area, Pore size distribution, Sorption energy

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Biochar, a carbon-rich material produced from biowastes through pyrolysis, has emerged as a promising material due to its unique structural characteristics, such as high surface area, porosity, and tunable surface chemistry. These properties make it suitable for various environmental applications, including carbon sequestration, water purification, and as a catalyst support. However, accurately characterizing biochar's adsorption properties poses significant challenges due to its complex and heterogeneous structure [1]. In this study, we investigate the surface properties of biochar using gas adsorption techniques, focusing on CO_2, N_2, and water vapor adsorption. We aim to evaluate key parameters such as surface area, pore size distribution, and sorption energy. The adsorption isotherms obtained allow us to compare the material's performance under different conditions and provide a detailed understanding of its adsorption behavior. The results of this study contribute valuable insights into the structure–adsorption relationship of biochar, aiding in the development of more efficient applications in environmental and industrial fields.

References

[1] Sigmund, G., Hüffer, T., Hofmann, T., Kah, M., *Sci. Total Environ.* 580, 770–775 (2017).

Quantification of the Pore Connectivity in Mesoporous Carbons by Analyzing Hysteresis Scanning Curves

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Keywords: mesoporous, hysteresis loop, gas adsorption

A thorough understanding of the nanopore architecture of materials is an essential factor for controlling various processes (e.g., mass transfer, percolation, pore blocking) in their applications. High resolution gas adsorption/desorption isotherms is a well-established and valuable tool for the characterization of nanoporous materials in the full micropore and mesopore range. While the techniques for the characterization of microporous materials are fairly well established, the assessment of the mesoporosity is still a challenge [1-3]. For such mesoporous materials, additional information about the pore network, its connectivity and pore size distribution can be extracted by a deep analysis of the hysteresis loop of the gas adsorption isotherms, which has led to numerous experimental and computation studies. In this context, we have analyzed the nanoporosity of mesoporous carbons by recording the high resolution gas adsorption isotherms of various probes (e.g. N_2, Ar, CO_2), performing scanning curves of the hysteresis loops. By applying different models for data interpretation and using a differential integrated approach in the partial and full hysteresis loops we have quantified the connectivity in the mesoporous network, and/or the presence of pore-blocking effects.

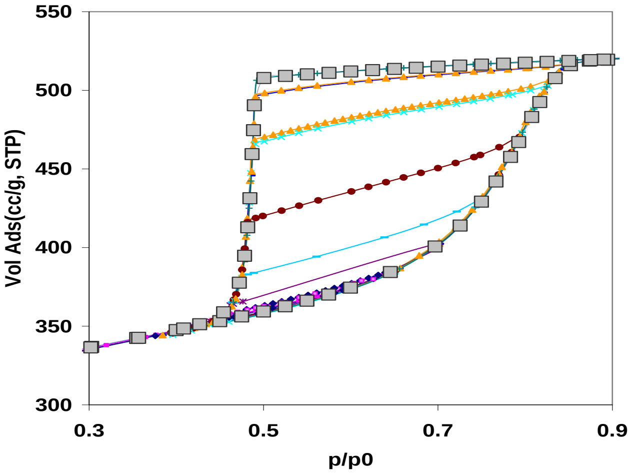

Figure 1. Descending scanning curves of the N_2 adsorption/desorption isotherm at 77K of a mesoporous carbon.

Acknowledgments. This work has received funding from the European Research Council (ERC) through the Consolidator Grant program under the grant agreement Nº 648161.

References

[1] F. Rouquerol, J. Rouquerol, K.S.W. Sing, P. Llewellyn, G. Maurin, Adsorption by Powders and Porous Solids, Elsevier, 2014.
[2] P.A. Monson, Understanding adsorption/desorption hysteresis for fluids in mesoporous materials using simple molecular models and classical density functional theory, Microp. Mesop. Mater. 160, 47-66, 2012.
[3] Wang Z, Huang J, Jiang G, Ji T, Lin H, Mu L, Zhu J. Quantification of Pore Connectivity in Hierarchically Porous Carbon by Percolation Effect Integrated Differential Hysteresis Scanning, Chem. Mater. 37, 4, 1337–1348, 2025.

Pilot-Scale Investigation of LNAPL Transport under Dynamic Water Table Conditions: 3D Three-Phase Flow Experiments and Simulations

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Keywords: Light non-aquous phase liquid (LNAPL), Time domain reflectrometer (TDR), Three-phase flow in porous media, water table fluctuations, Pilot scale

Light Non-Aqueous Phase Liquids (LNAPLs), such as diesel fuel, are a persistent source of subsurface contamination, challenging environmental assessment and remediation efforts [1]. This study presents a comprehensive investigation of LNAPL migration and redistribution in both saturated and unsaturated zones through large-scale pilot experiments and three-phase flow simulations. Conducted in the 5.2 × 3.6 × 3.6 m^3 PluriMetric Pilot (PMP) tank, the experiments simulate realistic field conditions, including intermittent diesel spills, water table fluctuations, and pumping interventions. The system was instrumented with multiple injection and pumping wells, piezometers, and Time Domain Reflectometry (TDR) probes to track phase distributions and monitor relative permittivity variations in the soil.

The experimental results reveal the dynamic behavior of LNAPL: initially forming a localized accumulation above the water table, then redistributing into a flatter layer influenced by capillary forces and gravitational drainage. Water table fluctuations—through imbibition and drainage cycles—promoted partial LNAPL entrapment and mobilization, while pumping experiments generated cones of depression and facilitated partial recovery of mobile LNAPL. TDR data effectively captured saturation trends, showing low permittivity values in air- and LNAPL-dominated zones and highlighting redistribution during water level changes.

Numerical simulations were developed by coupling the continuity equation with a generalized form of Darcy’s law, incorporating Stone I and van Genuchten-Mualem models to describe multiphase flow [2]. The model accurately reproduced LNAPL-air and LNAPL-water interface dynamics and integrated a permittivity mixing model that closely matched experimental TDR data across different tank regions.

This integrated experimental–numerical approach enhances the understanding of LNAPL behavior under transient hydrodynamic conditions and supports the development of improved remediation strategies. The results provide valuable guidance for optimizing well placement, pumping regimes, and monitoring protocols. Future work should explore the impact of subsurface heterogeneity and test alternative remediation techniques to refine predictive models and boost LNAPL recovery efficiency in complex geological settings.

References

[1] Koohbor, B., Colombano, S., Harrouet, T., Deparis, J., Lion, F., Davarzani, D., & Ataie-Ashtiani, B. (2023). The effects of water table fluctuation on LNAPL deposit in highly permeable porous media: A coupled numerical and experimental study. Journal of Contaminant Hydrology, 256, 104183.

[1] Stone, H.L., 1970. Probability model for estimating three-phase relative permeability. Journal of petroleum technology 22, 214–218.

Impact of water table fluctuations on the redistribution of light hydrocarbons in heterogeneous porous media

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Keywords: Dynamic capillary pressure, multiphase flow, Light non-aqueous phase liquids

1. Introduction

Contamination of the subsurface environment by light petroleum hydrocarbons is rather often due to the widespread consumption of such products. These pollutants characterised by toxicity and low solubility with water pose risks for ecosystems as well as human health. Understanding the fate and transport of these products after their release into the subsurface is essential for the future remediation strategies. After being released into the subsurface, pollutant moves towards the subsurface up to the groundwater level, where it undergoes significant redistribution due to the change of the groundwater level. Taking into account the water table fluctuations is vital for proper management of the contaminated area. We conducted a laboratory experimental study to investigate the impact of water table fluctuations, soil heterogeneity, and pollutant type on contaminant redistribution at the interface between the saturated and unsaturated zones. Main purpose of the experiment is to characterize the light hydrocarbons redistribution under water table fluctuation using geophysical sensors (TDRs), image analysis and further testing the remediation agents presented in the field.

2. Methodology

Experimental setup consisted of a 1D column made of PVDF (65 cm height and 10 cm inner diameter), with the glass window on the frontal part allowing to visualisation of the experiment 1. The column has four ports for time domain reflectometers (TDRs) and two pressure ports at each line with TDRs, allowing to take the measurements of the relative permittivity and the pressure simultaneously. Preliminary test with heterogenous structure has been performed with one cycle of imbibition-drainage followed by further surfactant and polymer plus surfactant flushing. Diesel oil from the gas station has been used as a light hydrocarbon representative. Porous media consisted of two grain size ranges of silica sand: 0.6-0.8 mm as fine sand and 1-1.25 mm as coarse sand. The column simulates three different zones of a deep subsurface soil: a water-saturated zone corresponding to the aquifer, a hydrocarbon zone as a supernatant pollutant floating above the water table, and an unsaturated soil zone. During the test, TDR data were recorded, and relative permittivity values were converted to saturation values using the complex refractive index model for the three-phase flow. Surfactant sodiumdodecyl sulfate (Sigma Aldrich) with the concentration of 5 g/L and bio-ploymer xanthan gum with the concentration of 1 g/l were used as flushing agents. It starts with the displacement of the non-wetting phase by the wetting phase (imbibition), followed by drainage (reverse process). The column experiments involved testing various heterogeneity configurations, including horizontal and vertical layered heterogeneities and drainage-imbibition intensity, in order to mimic the site conditions. Additionally, a complex mixture of degraded hydrocarbons from a pilot site is being tested.

3. Summary of findings

Preliminary tests showed higher value for the residual diesel saturation and effect of hysteresis in smear zone of three-phase flow, leaded by higher capillary forces. The heterogeneity of porous media

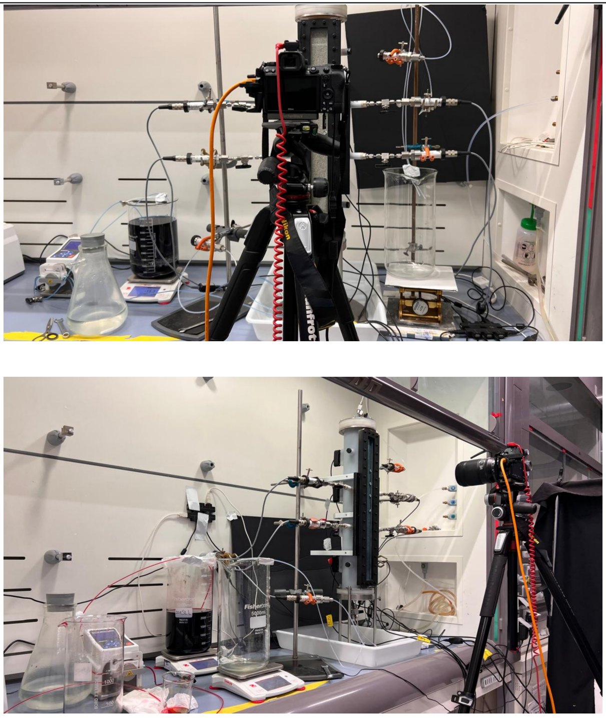

Figure 1: Caption

plays a crucial role in the redistribution of light hydrocarbons during drainage and imbibition processes. This factor must be carefully considered in the design of effective remediation strategies. The entry pressure of porous media, which is typically higher for smaller pores due to stronger capillary forces associated with reduced pore diameter, plays a key role in driving the redistribution of hydrocarbons towards higher permeability zones. This phenomenon contributes to lower residual saturation levels in the medium. Ongoing experiments are planned to give more insights about complex fluid distribution, due to its higher viscosity compared to diesel and the different components pathway and the hysteretical behaviour observed with diesel will not be retained. These results will be presented during the presentation of this work.

Modeling of the Hydrophobic Treatment of Gas Diffusion Layers to predict PTFE distribution

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Keywords: fibrous material; colloidal dispersion; drying; numerical modeling

Proton Exchange Membrane Fuel Cell (PEMFC) is currently considered as a pollutant-free alternative to thermal engines, especially for Heavy Duty applications. The Gas Diffusion Layer (GDL) is a crucial component ensuring heat, electrical, and mass transports thanks to its carbon porous structure [1]. GDL also plays a major role in the water management by ensuring a trade-off between drying (too low water vapor content) and flooding (too high liquid saturation).

To reduce the flooding risk during PEMFC operation, a hydrophobic treatment is applied to the GDL. The porous carbon material is dipped into a colloidal dispersion of PTFE then dried and sintered. As it can be seen in Figure 1, the PTFE particles do not coat uniformly the GDL fibres. The PTFE distribution actually depends on the drying conditions [2]. Interestingly, an 'optimized' PTFE distribution is still an open question and progress on this matter will help improving GDL. Currently, the most advanced GDL models consider 3D volumes representing its microstructure, which are obtained from X-ray microtomography or randomly generated. However, PTFE is either not taken into account, as it is not visible in X-ray tomography, or it is numerically added by morphological opening [3] for which the deposition criteria are questionable.

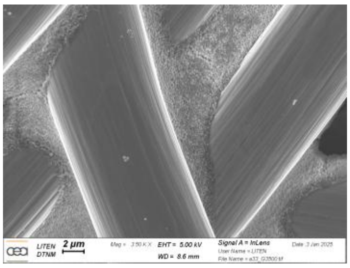

Figure 1: SEM image of the GDL after being dipped in the PTFE dispersion and dried

Based on characterizations of the hydrophobic ink and on SEM observations to locate the PTFE, a model of the drying of the colloidal dispersion in the GDL is developed, to simulate the final PTFE distribution in the microstructure. Numerical results are compared to cross-section distributions of PTFE in the GDL obtained by SEM-EDX for different drying conditions. experimental. Numerical results are also compared to experimental distributions obtained on model carbon porous microstructures.

This research is part of the project “DECODE" which has received funding from the European Union’s Horizon Europe research and innovation program under grant agreement N° 101135537. More information on the project can be found at www.decode-energy.eu.

References

[1] Ozden et al. « A Review of Gas Diffusion Layers for Proton Exchange Membrane Fuel Cells». *Progress in Energy and Combustion Science*, Vol. 74, 50-102, (2019).
[2] Mathias et al. « Diffusion media materials and characterisation». *Handbook of fuel cells—fundamentals, technology and applications*, Vol. 3, 517–537, (2003).
[3] Fadzillah et al. « Review on microstructure modelling of a gas diffusion layer for proton exchange membrane fuel cells ». *Renewable and Sustainable Energy Reviews*, Vol. 77, 1001-1009, (2017)

Modeling Groundwater Flow In Unconfined Aquifers With Physics-Informed Neural Networks: Inverse Modeling

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Keywords: Physics-Informed Neural Networks, Groundwater Modeling, Inverse Problem

Accurate groundwater modeling plays a vital role in managing subsurface water resources, particularly in heterogeneous aquifers where flow dynamics are complex, and data availability is limited. Traditional physics-based models are often computationally expensive for large-scale or highly variable domains. Data-driven models are more efficient from a computational point of view, but they require a large amount of data and have limited reliability when used for predicting conditions outside the training data. Recent advancements in machine learning have introduced Physics-Informed Neural Networks (PINNs) as a promising alternative that combines advantages of physics-based and data-driven models. By incorporating physical laws directly into the training process, PINNs enable the development of models that remain physically consistent even with sparse data.

This study investigates the application of PINNs for modeling groundwater flow in an unconfined aquifer with spatially varying hydraulic conductivity. Synthetic datasets are generated using COMSOL Multi-physics and serve as reference solutions for training and validation. To evaluate the robustness of PINNs in data-scarce conditions, portions of the training data are deliberately omitted, encouraging the model to rely more heavily on the embedded governing equations.

Furthermore, due to the practical difficulties and high cost associated with measuring aquifer parameters in the field—such as hydraulic conductivity and storage coefficients, this research explores the use of PINNs for inverse modeling. By leveraging their physics-based structure, PINNs are employed to infer unknown subsurface parameters from limited observations while preserving consistency with physical laws. This approach offers a viable alternative to traditional calibration methods that typically require extensive field measurements and dense datasets.

Future work will focus on extending the methodology to real-world scenarios characterized by complex boundary conditions and irregular domain geometries, aiming to assess the potential of PINNs for practical applications in challenging hydrogeological settings.

Direct Experimental Quantification of Salt-Induced Permeability Reduction in Porous Media

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Keywords: Salt precipitation, Porous media, Permeability reduction, X-ray tomography

Salt crystallization is a known issue during subsurface gas injection, particularly in the context of supercritical CO_2 injection into saline aquifers. Field observations have confirmed that salt precipitation can significantly reduce permeability and injectivity. Experimental studies reproducing such conditions have reported permeability reductions ranging from 10% to 83% [1], highlighting the severity of pore clogging by salt. Similar phenomena have also been observed during gas production operations [2]. Most laboratory investigations rely on drying under reservoir temperature conditions, typically resulting in localized crystallization within the pore structure. However, other studies suggest that under certain subsurface conditions, particularly at high flow rates, a more uniform salt precipitation pattern can occur [3]. In this study, we aim to experimentally reproduce such homogeneous salt distribution using a controlled vacuum drying protocol. We use both model porous media (VitraPOR cylinders, 6 mm in diameter, with pore sizes of 40–100 µm, 100–160 µm and 160–250 µm) and natural rock samples (Bentheimer and Vosges sandstone, and Savonnières limestone). The protocol consists of repeated cycles of imbibition with a saturated KCl solution, followed by vacuum drying, leading to progressive salt accumulation. After every three cycles, X-ray tomography and mass measurements are performed to quantify in-pore salt deposition and salt distribution, and the sample's permeability is measured using a Hassler cell. This protocol allows for the establishment of a direct experimental relationship between permeability and salt mass, simultaneously assuring a homogeneous salt distribution. Our results show that vacuum drying enables uniform salt precipitation throughout the pore network, with salt consistently accumulating in the same regions. Such homogeneity was not achieved using conventional drying methods, which typically induce heterogeneous crystallization, mostly at sample edges, thereby making it difficult to derive an accurate permeability-salt relationship. First observations on the VitraPOR samples with 40–100 µm pores reveal an exponential permeability decline as salt mass increases. This experimental framework is highly relevant to subsurface injection scenarios and offers a rare direct quantification of permeability loss due to homogeneous salt precipitation at the REV scale, an effect that is usually estimated only through empirical models in the literature. As such, the experimental dataset can be used to validate or refine those models.

Acknowledgements: The authors acknowledge the support from the ERC Starting Grant PRD-Trigger (grant agreement N° 850853).

References

[1] N. Muller, R. Qi, E. Mackie, K. Pruess, and M. J. Blunt, CO_2 injection impairment due to halite precipitation, *Energy Procedia, 1*(1), 3507–3514 (2009).
[2] X. Yang et al., Mechanism of salt precipitation blockage in low-producing gas wells and the method of acidification blockage removal, *ACS Omega, 9*(9), 10886–10896 (2024).
[3] L. Sun et al., Salt precipitation and pore structure changes during CO_2 injection into porous media, *J. Clean. Prod.*, 505, 145446 (2025).

Assessment of Groundwater Vulnerability to Leachate Contamination Using Hydrodynamic and Geochemical Indicators in Belloua Mountain, Kabylia, Algeria

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Keywords: porous media, groundwater vulnerability, leachate dispersion

The uncontrolled discharge of solid waste and domestic effluents in mountainous rural areas is a growing environmental concern. In Kabylia (Northern Algeria), the Belloua massif represents a fractured metamorphic aquifer system highly vulnerable to anthropogenic pressures and climate change. This study presents a coupled hydrogeological and geochemical approach to evaluate the vulnerability of groundwater to leachate migration from ancient landfills. In-situ measurements (pH, EC, ORP, T°), laboratory analyses (major ions, nitrates, ammonium, and DOM by 3D fluorescence), and geological mapping were combined to characterize flow paths and contaminant dispersion in porous fractured media.

A hydrogeological conceptual model was established, integrating fracture networks and geomorphological factors. The results highlight three zones with contrasting vulnerability levels. High nitrate and phosphate levels, and the detection of anthropogenic DOM fluorescence signatures, confirm pollution risks. Ion exchange patterns (Na^+/Ca^{2+}, K^+/Mg^{2+}) suggest strong water–rock interactions enhanced by leachate infiltration. The spatial distribution of contaminants correlates with fracture density and topographical convergence, pointing to preferential flow in subsurface pathways. This study emphasizes the importance of multi-parameter monitoring and modeling for the reactive transport in porous media, supporting water resource protection policies in mountainous environments.

References

[1] Slimani M. et al., "Multivariate assessment of groundwater pollution near landfills", Journal of Hydrology, 610, 127984 (2022).

[2] Zouhri L. et al., "Hydrogeochemical behavior of contaminated aquifers", Environmental Earth Sciences, 76, 385 (2017).

[3] Kourgli A. et al., "Application of DRASTIC and GIS to assess groundwater vulnerability", Arab J Geosci, 12, 336 (2019).

Coupled heat and moisture transfer in porous building materials: accounting for the sorption hysteresis

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Keywords: Hysteresis, porous media, heat and moisture transfer

Abstract

The use of highly porous (~70%) bio-based materials enhances indoor environmental conditions by favorising heat and mass transfer, due to their porous and multiphase structure. However, the modeling of coupled heat and moisture transfer is often less accurate due to the negligence of adsorption/desorption hysteresis phenomena.

$$\begin{cases} \rho_s C_m \dfrac{\partial RH}{\partial t} = div\big((K_l^l + K_l^v)\nabla RH + (K_T^l + K_T^v)\nabla T\big) \\ \rho_s C_p \dfrac{\partial T}{\partial t} = div(\lambda^* \nabla T + \chi \nabla RH) \end{cases} \tag{1}$$

This research investigates the integration of hysteresis effects into hygrothermal transfer models using the Carmeliet model [1], based on Mualem model, fully implemented within Comsol Multiphysics software. In this approach, the hysteresis model is coupled with the hygrothermal transfer equations (equation (*1*)) through the moisture storage capacity (equation *(2)*), which is calculated from the water content (equation *(3)*). Experimental validation conducted in a bi-climatic chamber (figure 1a) reveals that accounting for hysteresis reduces the discrepancy between simulation and experimental measurements from 6% to 2% (figure 1b), highlighting the significance of this parameter for ensuring model accuracy and reliability.

$$C_{m\,ads,hys} = \frac{\partial W_{ads,hys}}{\partial RH} \tag{2}$$

$$W_{ads,hys}(RH) = W_i + \big(W_{ads}(RH) - W_{ads}(RH_i)\big).\frac{W_{sat} - W_{des}(RH_i)}{W_{sat} - W_{ads}(RH_i)} \tag{3}$$

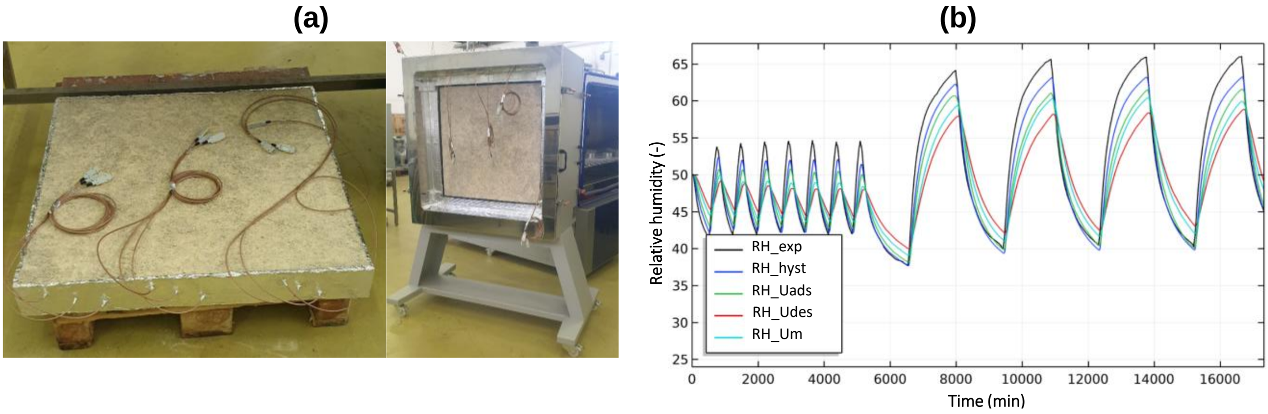

Figure 1: (a) Hemp concrete wall with sensors; (b) Relative humidity: experimental data vs simulations with/without hysteresis.

References

[1] J. Carmeliet, M. De Wit, H. Janssen, Hysteresis and moisture buffering of wood. 7th Nordic Symposium on Building Physics, Reykjavik, Islande (2005).

Synthesis and characterization of nickel oxide nanoparticles by the PECHENIN method for Corrosion Protection and Porous Material Reinforcement Applications

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Keywords: *Nanoparticules, NiO, DRX, FX,SEM, porous media, material protection*

Abstract

This study aims to develop high-purity nickel oxide (NiO) nanopowders in the laboratory using the PECHENIN method, with the goal of applying them as corrosion inhibitors and as reinforcement agents for porous materials. Nickel oxide was synthesized from a nickel nitrate solution, treated with citric acid and ethylene glycol under agitation at 80 °C, with pH adjusted to 8. A greenish gel was formed and subsequently dried in an oven at 100 °C for 24 hours to remove volatile solvents.

X-ray diffraction (XRD) analysis revealed an amorphous phase without distinct mineral structures, characteristic of unalloyed nickel coatings. The most prominent diffraction peaks were identified along the planes (17.54692), (11.65564), (9.03758), (6.80638), and (5.05080). X-ray fluorescence (XRF) analysis showed a predominant composition of nickel oxide (NiO) with 98.5% purity, and trace amounts of Na, Mg, Si, and Al.

These synthesized nanoparticles present strong potential for integration into porous matrices (e.g., concrete, ceramics, composites) as active anticorrosive agents. Their high reactivity and surface area enhance protection in aggressive environments and improve the mechanical integrity of porous structures. Incorporating NiO into porous barrier systems offers a promising strategy for corrosion resistance and functional reinforcement in environmental and civil engineering applications.

Reference examples:

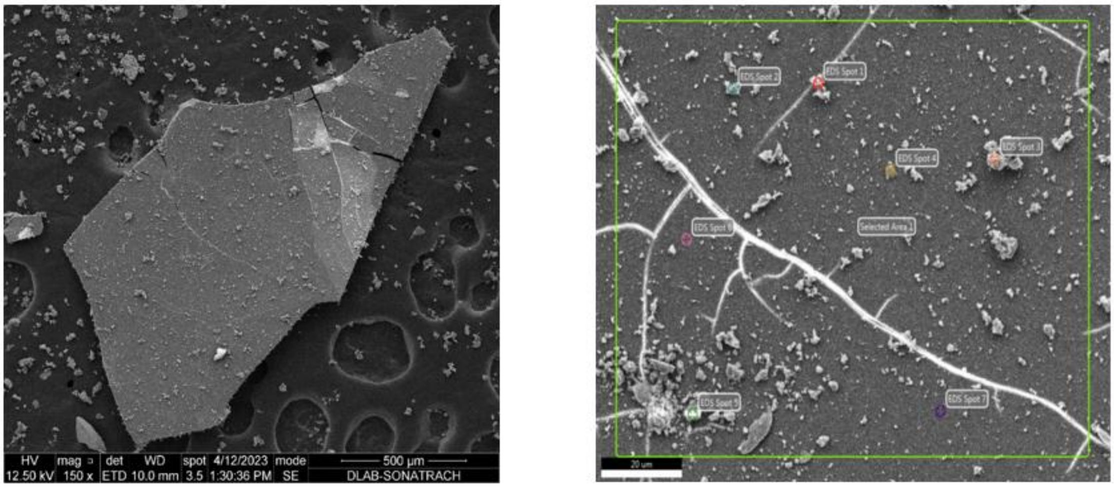
[1],Stark, W.J., et al., Industrial applications of nanoparticles. Chemical Society Reviews, 2015. 44(16): p. 5793-5805.
[2],Kim, B.H., et al., Synthesis, characterization, and application of ultrasmall nanoparticles. Chemistry of Materials, 2014. 26(1): p. 59-71.
[3],Dong, F., et al., Nanomaterials for environmental applications. 2014, Hindawi.

Table example:

Elément	%of mass	% atomique	Total Intensity	%error
O	**25.68**	**40.24**	**59.26**	**17.74**
Ni	**42.01**	**49.41**	**192.99**	**12.27**
C	**32.31**	**10.36**	**76.50**	**14.30**

Table 1: Results of the Zone 1 qualitative and quantitative analysis

Figure example:



Zone -01 -

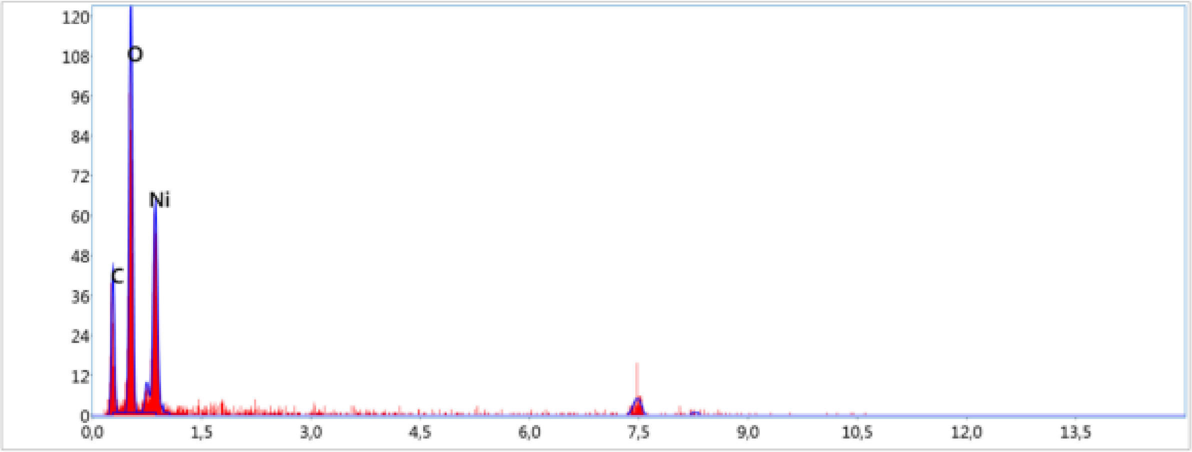


Figure 1: Scanning electron microscope images of samples of NiO nanoparticles zone 1 and his qualitative and quantitative analysis spectrum

References

[1] Crooks R M, Zhao M, Sun L I, Chechik V and Yeung L E E K 2001 Dendrimer-Encapsulated Metal Nanoparticles : Synthesis , Characterization , and Applications to Catalysis 34 181–90

[2] Sahu, K. K. Nanda and S. N. Photoluminescence of CdS nanocrystals:. effect of ageing Solid State Communications. (1999)671, Vol. III, 12.

[3] Les nanoparticules: Un enjeu majeur pour la santé au travail ?, Les Ulis: EDP Sciences, 2007. https://doi.org/10.1051/978-2-7598-0319-4

Field scale Thermo-poro-mechanical modelling for CO_2 storage

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Keywords: Field scale, geomechanics, Temperature, CO2 Storage, Multiphysics integrity

The Aramis CO2 storage project in the Netherlands, specifically on the L4-A field, has been the subject of extensive geomechanical assessment. The key geological routes for migration of CO2 outside of the storage complex include fracturing the caprock and migration along reactivated faults/fractures within the storage complex. These mechanisms are controlled by the in-situ stresses, pressures, and temperatures in the reservoir and caprock, as well as injection pressures at the wells.

The first part will deal with the field scale geomechanical modelling workflow. A field scale model was constructed to include the storage complex and the sedimentary pile, using surfaces, faults. The field-scale model was populated with petrophysical and geomechanical properties. The workflow assessed the stress initialization, impact of the depletion in the field then simulated the injection of CO2 for 20 years, and 180 years post injection. The impact of the pressure and temperature changes on both the reservoir and the caprock were assessed to understand the following key risks: risk of loss of containment due to caprock fracturing, risk of loss of containment due to reactivated fault permeability enhancement in the field, risk of induced seismicity with CO2 injection. The study also evaluated the ground deformation (compaction/subsidence).

The second part introduces GEOS, an innovative multiphysics tool currently under development. A flow model, matching the historical production period, was employed to generate historical pressure changes in the reservoir during production and expected pressure and temperature. The new GEOS model is compared with the previous operational results to evaluate the accuracy and reliability of the geomechanical modelling. This includes comparing predicted and observed pressure changes, temperature changes, stress changes and the occurrence of injection-induced hazards. The comparison also assesses how accurately the models represent the complex geological structures of the Aramis field, and how this affects the accuracy of its predictions.

References

[1] Aramis CO2 storage Case Study – A Geomechanical Assessment of ... - SSRN. https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4282320.
[2] Netherlands: TotalEnergies, Shell Netherlands, EBN and Gasunie Form .... https://totalenergies.com/media/news/press-releases/partnership-to-develop-aramis-offshore-ccs-project.
[3] CO_2 Specifications for Aramis transport infrastructure. https://www.aramis-ccs.com/news/co2-specifications-for-aramis-transport-infrastructure.
[4] Aramis CCS | Homepage. https://www.aramis-ccs.com/.

Experimental Characterization of Foam Flow and Gas Trapping in Porous Media

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Keywords*:* Foam flow, TDR probes, porous media

This study aims to better characterize the process of foam flow in porous media in order to develop innovative remediation strategies for polluted soils and aquifers. One of the key effects to enhance light non-aqueous phase liquid (LNAPL) recovery using foam injection lies in the homogenization of displacement fronts associated with the high apparent viscosity of foam (several hundred to several thousand times that of water). The apparent viscosity tends to increase with the gas fractional flow, f_g , up to a maximum, beyond which the foam is believed to become unstable. Conversely, it tends to decrease with increasing capillary number *Ca*, indicating strong shear-thinning behavior. These trends have been previously reported in several studies for various porous media, but the underlying small-scale mechanisms remain poorly understood. Recent microfluidic approaches that mimic porous media have reproduced the main features of foam flow [1] and revealed that the flow is concentrated along preferential pathways, depending on *Ca* and f_g. Optical observation revealed that immobile trapped foam could be bypassed by the flow. Moreover, effective viscosity was found to be proportional to f_g /Ca, a behavior interpreted as resulting from quasi-static bubble deformation through constrictions.

The current study aimed to extend these observations to realistic 3D porous media. An original column setup was developed to study foam flow. It was designed to monitor not only gas and total mass flow rate and pressure drop but also volumetric water and gas content using Time Domain Reflectometry (TDR) probes. It was also designed to allow optical access to the porous media. To our knowledge, this is the first experimental setup that enables simultaneous and direct measurement of both phase saturation and pressure gradients. Results obtained on a well graded homogeneous sandpack over a wide range of f_g and *Ca* semi-quantitatively confirm in 3D the findings of Mauray et al. [1], particularly regarding the pressure drop induced by foam flow. The water saturation measurements yield striking results: depending on the flow regime, the volumetric gas fraction can significantly exceed the injected gas fractional flow f_g , suggesting considerable gas trapping and highly heterogeneous flow patterns.

References

[1] A. Mauray , M. Chabert, H. Bodiguel, *Phys. Rev. Fluids,* 5, 094004 (2020).

Optimizing Surfactant Foam Formulations for Enhanced (Bio)Remediation of Petroleum-Contaminated Soil

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Keywords: soil contamination, petroleum hydrocarbons, surfactant foam, foam stability, bioremediation

Abstract. Soil contamination by petroleum hydrocarbons remains a significant environmental issue due to the toxicity, persistence, and mobility of these compounds. Bioremediation has emerged as an environmentally friendly and cost-effective approach that uses microorganisms to degrade hydrocarbons into less harmful substances [1]. However, its efficiency is often constrained by the low bioavailability of microorganisms, their uneven distribution in the subsurface, and the heterogeneous nature of soil structure, which hinders microbial transport and nutrient accessibility. Foam-based (bio)remediation technologies have shown promise in overcoming these limitations by acting as carriers for microorganisms and nutrients [2,3]. Besides mobilizing contaminants, foams allow for more uniform delivery of remediation agents, increasing contact with contaminants. Foam effectiveness depends on key physical properties – particularly generation, foamability, stability [4]. These factors influence transport behaviour and microbial delivery, particularly in the presence of hydrophobic compounds such as hydrocarbons.

This work aims to evaluate environmentally friendly and cost-effective surfactant formulations to produce stable foams suitable for microbial transport. Surfactant selection is critical: biosurfactants such as rhamnolipid and saponin offer low toxicity and high biodegradability, but are relatively expensive. In contrast, synthetic surfactants like Sodium Dodecyl Sulfate (SDS), Tween 80 and Triton X-100 are more accessible but potentially less sustainable. The semi-synthetic, zwitterionic surfactant Cocamidopropyl Betaine (CAPB) represents an intermediate profile between sustainability and performance. We investigate single (control), binary, and ternary surfactant formulations at a total concentration of 0.5% w/v using the Dynamic Foam Analyzer (DFA-100, Krüss) to assess foamability, stability (half-life), and bubble size under ambient conditions. Preliminary results are promising, and a full comparative analysis of the formulations will be presented at the conference. Future work will involve foam injection in porous media to evaluate microbial transport and delivery efficiency for enhanced bioremediation.

References

[1] Pande, V., Pandey, S. C., Sati, D., Pande, V., & Samant, M., Bioremediation: an emerging effective approach towards environment restoration. *Environmental Sustainability*, 3, 91-103 (2020).

[2] Bouzid, I., Herrera, D. P., Dierick, M., Pechaud, Y., Langlois, V., Klein, P. Y., ... & Fatin-Rouge, N., A new foam-based method for the (bio) degradation of hydrocarbons in contaminated vadose zone. *Journal of Hazardous Materials*, 401, 123420 (2021).

[3] Jeong, S. W., Jeong, J., & Kim, J., Simple surface foam application enhances bioremediation of oil-contaminated soil in cold conditions. *Journal of Hazardous Materials*, 286, 164-170 (2015).

[4] Baigadilov, A., Colombano, S., Omirbekov, S., Cochennec, M., Davarzani, D., Lion, F., ... & Bodiguel, H., Surfactant foam injection for remediation of diesel-contaminated soil: A comprehensive study on the role of co-surfactant in foaming formulation enhancement. *Science of The Total Environment*, *930*, 172631 (2024).

Semi-analytical solution for flow with time-varying viscosity in fractured porous media

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Keywords: Variable viscosity models; fractured porous media; semi-analytical solution; numerical model validation

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Some polymer solutions can form a gel when injected into a porous medium. These gel-forming solutions are of great interest for specific applications such as improving the geotechnical characteristics of soil, and enhancing the recovery of contaminants or oil from fractured reservoirs. During its travel through porous media, the viscosity of the gelling solution increases, which can significantly affect its hydraulic properties. Variable viscosity flow in the two fractures can be described by the steady-state mass conservation equation (1) and the Darcy's law (2), respectively (Younes et al., 2024):

$$\nabla . V = 0 \tag{1}$$

$$V = -\frac{k}{\mu} \nabla P \tag{2}$$

where P is the pressure [Pa], V is the Darcy velocity [LT^{-1}], μ is the fluid dynamic viscosity [$ML^{-1}T^{-1}$], k is the permeability of the fracture [L^2], and ∇ represents the gradient operator.

This work considers the injection of a gelling polymer into a system of two fractures with different apertures as depicted in fig 1. The viscosity of the injected fluid varies in time according to equation (3).

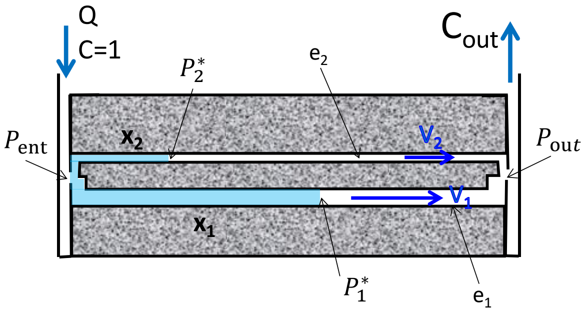

Figure 1: Conceptual framework of the test case.

$$\mu_1(t) = a_1 + a_2 e^{a_3 t} \tag{3}$$

In this study, a semi-analytical solution has been developed to solve the problem depicted just before, which is characterized by three phases occurring during the injection process. The first phase occurs until the gelling solution entirely fills the large fracture. In this phase, the velocity inside the large fracture diminishes, while, by compensation, it increases in the thin fracture. Then, the second phase occurs until the thin fracture becomes fully invaded by the injected solution. During this phase, the velocity in the large fracture increases, and that of the thin fracture decreases. Finally, the last phase occurs when both fractures are saturated by the injected gelling solution. During this last phase, the velocity inside the large fracture continues a slight increase, while it slightly decreases in the thin fracture for the case of time-varying viscosity. Our semi-analytical solution allows validating a numerical scheme. Hence we demonstrate a good agreement between them with minor discrepancies observed.

References

[1] Younes, A., Rajabi, M. M., Rezaiezadeh Roukerd, F., & Fahs, M. An analytical solution for variable viscosity flow in fractured media: Development and comparative analysis with numerical simulations. Water Resources Research, 60(3), e2023WR035741. (2024).

Free Surface Flow around and Inside an Amphiphilic Porous Hollow Fiber

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Keywords: porous fiber, interface process, amphiphilic matter, wettability, free energy, free surface flow

The issue of flow along porous microtubes arises in many industrial contexts, particularly in the case of hollow fiber membranes. These can be made of organic material (cellulose) which has an amphiphilic character. Flow in a microtube has been the subject of many studies in the case of an impermeable wall. Recently, we focused on the wettability effect by studying microtube with thin film in inertialess limit [1, 2]. We have highlighted many flow regimes specific to partial wetting. Notably, traveling waves of drop train that consists of a clustering of drops without coalescence. However, little has been done in the case of a porous wall.

The objective of this article is the modelling and the simulation of film flow dynamics inside and over a narrow tube of a porous wall and driven by a longitudinal force as the gravity. Due to amphiphilic properties of the hollow fiber, Darcy's model no longer yields and a free energy based model as to be considered in the wall [3]. Moreover, according to [4], flows are not only hydrodynamically but also thermodynamically coupled. We propose to combine the hydrodynamic model of [1] for the free surface flows over the fiber with the approach developed in [3, 4] for water exchange between thin films and the porous wall. We associate to each medium a free energy functional depending on the order parameter
in each medium (thin liquid films and porous medium). Evolution equations are written in the form of a gradient dynamics for non-conserved order fields [5].

The simulation of axisymmetric thin film flows highlights complex interactions between the inside and outside flows notably due to the amphiphilic properties of the porous wall (Fig. 1). This rich behavior is analyzed using time integration, path-following methods, and numerical bifurcation analysis.

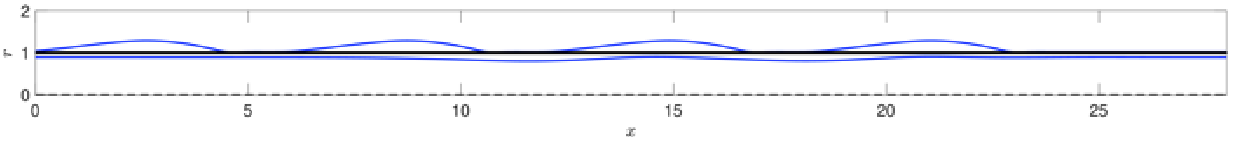

Figure 1: Radial profiles (blue line) of axisymmetric flow over and through the porous wall of a hollow fiber. The bold black line represents the porous wall. The driving force is horizontal.

References

[1] P. Beltrame, Partial and complete wetting in a microtube, EPL 121:64002 (2018).
[2] P. Beltrame, Drop train flow in a microtube, Eur. Phys. J. Spec. Top., 232(4), 435–442 (2023).
[3] P Beltrame and F. Cajot, Model of hydrophobic porous media applied to stratified media: Water trapping, intermittent flow and fingering instability, EPL 138:53004 (2022).
[4] F. Cajot, C. Doussan, S. Hartmann and P. Beltrame, Model of drop infiltration into a thin amphiphilic porous medium, J. Colloid Interface Sci. 684, 35–46 (2025).
[5] O. Kap et al., Nonequilibrium configurations of swelling polymer brush layers induced by spreading drops of weakly volatile oil, The Journal of Chemical Physics 158: 174903 (2023).

Theory and Lattice Boltzmann Modeling of Pollutants in Solution: Effect of the Porous Medium Heterogeneity on Adsorption and Transport

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Keywords: Adsorption, Transport, Emerging pollutants, Lattice Boltzmann Method

In recent years, a strong interest was shown by the large public for the impact and fate of new pollutants which are threatening the environment as well as human health [1, 2]. Consequently, in parallel to recent technical progress, large efforts in fundamental and applied research were devoted to this field. Many detection and remediation tools have been developed in the past years for emerging pollutants such as per- and polyfluoroalkyl substances (PFAS), pharmaceutical and personal care products (PPCP), antibiotics, etc. In addition to the role of numerous environmental parameters (pH, salinity, coexisting organic matter, ions, etc.), the chemical (*e.g.*, composition, molecular structure, dissociation) and physical (*e.g.*, phase diagram, solubility, aggregation) specificities of these complex molecules lead to a rich and intriguing behavior near solid surfaces [3, 4]. In this context, while adsorption-based solutions offer promising perspectives for efficient remediation approaches, their development is limited by significant knowledge gaps in the fundamental mechanisms governing the behavior of emerging pollutants in solution and near solid surfaces. By adopting a fundamental physical chemistry perspective, we develop a robust model that includes the effects of surface saturation, reservoir depletion, and lateral interactions on the adsorption kinetics and thermodynamics of PFAS molecules. More specifically, a thermodynamic framework that accounts for two- and three-body lateral interactions is built and the effect of each interaction parameter on the shape of the adsorption isotherm is investigated. Then, a thorough kinetic model based on the thermodynamics of adsorption and on a rigorous definition for the adsorption and desorption rates (which, in a general framework, should include surface saturation, reservoir depletion and lateral interactions) is developed. The latter is then implemented into Lattice Boltzmann simulations to numerically solve the transport equations governing the mass transfer of complex pollutants in bimodal porous media [5, 6]. These media serve as simplified yet effective representations of natural media such as soils or sediments as well as adsorption-based filtration systems. Our approach aims to characterize both the effects of dual porosity and topological heterogeneities of the media on the adsorption and transport mechanisms of emerging contaminants such as PFAS. Our approach provides new insights into the interplay between adsorption and transport mechanisms in heterogeneous media. As a long term perspective, the present work could pave the way for improved remediation strategies using porous filters and provide a deeper understanding of the impact of emerging pollutants on natural porous environments (*e.g.*, soils, sediments).

References

[1] European Comission, Comission regulation (EU) 2022/2388. (2022)
[2] Safer States, USA, Analysis of State Legislation Addressing Toxic Chemicals and Plastics. (2024)
[3] Ramona L Johnson et al., The adsorption of perfluorooctane sulfonate onto sand, clay, and iron oxide surfaces, Journal of Chemical & Engineering Data, 52.4, pp. 1165-1170 (2007)
[4] Sofia F Soares et al., Magnetic nanosorbents with siliceous hybrid shells of alginic acid and carrageenan for removal of ciprofloxacin, International journal of biological macromolecules 139, pp. 827-841 (2019)
[5] Irina Ginzburg, Goncalo Silva, and Laurent Talon, Analysis and improvement of Brinkman lattice Boltzmann schemes: Bulk, boundary, interface. Similarity and distinctness with finite elements in heterogeneous porous media, Physical Review E, 91.2, p. 023307 (2015)
[6] Zaineb Zaafouri et al., Lattice Boltzmann method for adsorption under stationary and transient conditions: Interplay between transport and adsorption kinetics in porous media, Physical Review E 104.1, p. 015314 (2021)

Experimental Study of Dissolution Patterns resulting from the competition between Forced and Solutal Convection

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Keywords: Experiments, buoyancy flows, pattern formation, dissolution, hydrodynamics

Landscapes on Earth's surface are shaped by erosion, whether mechanical or chemical. For instance, chemical erosion, or more specifically, erosion by dissolution, is the main mechanism for the erosion of limestone, gypsum and salt. During this process, topography, flow, and solute transport interact to generate regular patterns whose size and shape are believed to reflect past hydrodynamic conditions. As the fluid density increases with solute concentration, dissolution creates density gradients that generate solutal convection flows under the influence of gravity. External flow also affects the local dissolution rate by shearing the solute boundary layer. Consequently, we investigate at MSC the formation of dissolution patterns under the action of turbulent water flow in the laboratory using salt and gypsum plates. Specifically, we characterize the dissolution rate and pattern orientation depending on the strength of the imposed flow. In experiments with fast-dissolving materials, we effectively demonstrate that dissolution pattern shapes and orientation are clearly affected by the competition between forced and solutal convection.

References

[1] Martin Chaigne. PhD thesis. *“Érosion par dissolution à grand nombre de Reynolds : hydrodynamique, morphogenèse et propulsion*”, Université Paris Cité, 2024.

Impact of Inertia on the Stability of Two-phase Flow: a Pore-doublet Approach

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Keywords: pore-doublet models, Haines jump, inertia

Haine's jumps, or rheons, occur during drainage in porous media at low capillary number and are characterised by pinning of the interface at a constriction, before a quick and sudden invasion of the next pore-body. During the jump, the interface's speed is two to three orders of magnitude above the average invasion speed. This raises the question: can inertia, usually neglected during the invasion, play a role during those jumps? In this presentation, we will focus on Haines jumps and the potential impact of localized inertial events on two phase flows in porous media.

Microfluidic devices, also called micromodels or aquifer-on-chips, are designed to mimic the porous media and to allow for the direct observation of the fluid flow and interfacial dynamics. In this work, particular interest is given to pore doublets, whose geometry is composed of two parallel channels connected together at the inlet and the outlet. Their structure allows us to reproduce the different regimes that appear during the drainge of a porous media [1], as well as to study the pore's invasion mechanisms, such as Haine's jumps.

We developed a pore-doublet model consisting in a set of equations resulting from the integration of mass and momentum equations. The model accounts for inertia effects. Simulations are then compared with experiments. The developed model as well as the experimental data allows to better understand the impact of inertia during two-phase flow. We showed that, even for Reynolds numbers below one, after a jump, the menisci can oscillate around their stable positions. If these oscillations, caused by the inertia of the fluid, are important enough, they can help or inhib the next Haine's jump, altering the order in which the pores are invaded. This can turn a stable drainage, where both channels are drained simultaneously, to an unstable one where one pathway is preferentially invaded over the other. We show that inertia must be considered when the density ratio or the aspect ratio between the pore bodies and the constrictions is high.

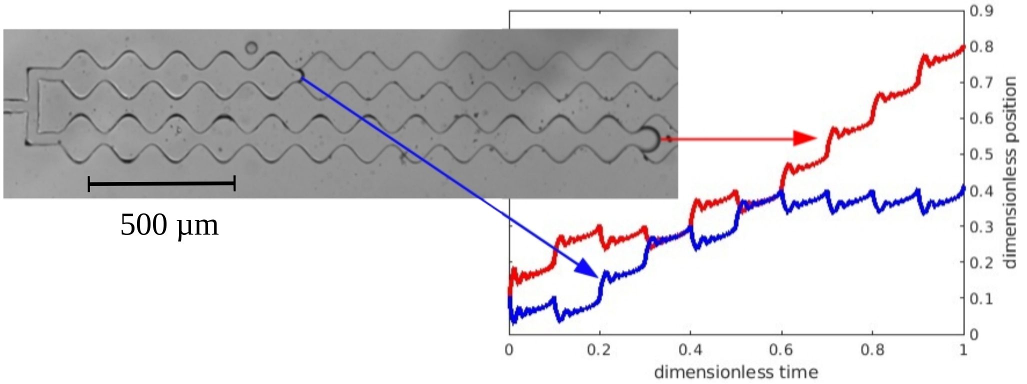

Figure 1: Experimental drainage compared with a numerical invasion. The blue and red curves show the interfacial dynamics, where inertia creates oscillations after the Haines jumps.

References

[1] Mansouri-Boroujeni *et al.* , How interfacial dynamics controls draingae pore-invasion patterns in porous media, Advances in Water Ressources, 171, (2023).

Multi-scale modelling of enzymatic hydrolysis of biomass using numerical homogenization

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Keywords: Biomass, Reactive Transport, Upscaling

The architecture of biomass is highly complex and varies from species to species: it can be defined as a continuum of spatial scales, from the scale of polymeric molecules making up plant cell walls (PCW) to the scale of plant tissues and organs (stem, leaves, etc.). These scales are highly interconnected and reflect not only the chemical and structural properties of biomass, but above all its reactivity to transformation processes such as chemical, physical, mechanical or biological reactions.

The aim of this project is to develop a homogenized model of enzymatic hydrolysis, one of the most widespread processes for converting lignocellulosic biomass in applications such as production of biofuels or bio-based chemicals. Existing models of enzymatic hydrolysis, including [1], do not consider the dual porosity structure of biomass, as illustrated in Figure 1.

In the present work, theoretical and numerical tools [2] are used to address this problem of diffusive and reactive transport in such a spatially heterogeneous porous medium. A numerical homogenization technique is developed to work on the scale of a fragment representative of a typical biomass (e.g. maize), while considering physical phenomena at lower scales. It is implemented on 2D image sets, currently for pure diffusive transport (Figure 2), before including the reactive component of the problem.

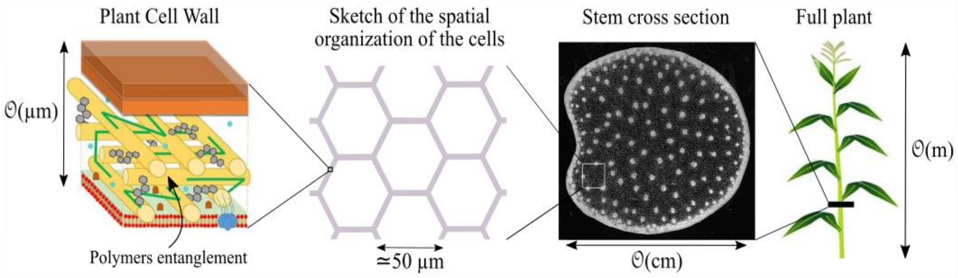

Figure 1: Maize, a porous material characterized by a continuum of spatial scales, adapted from [3]. The plant cell walls (a few microns thickness) consist in a porous entanglement of polymers (with pores in the nanometric size range). At the scale of a stem cross section, the material can be seen as a porous medium with the lumen cells as the pores (typically a few tens of microns).

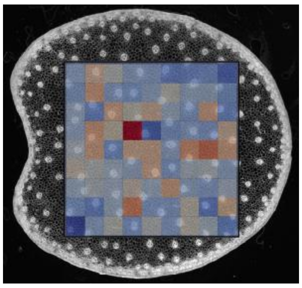

Figure 2: Illustration of the heterogeneities in equivalent diffusion coefficients, computed in the middle of the stem cross section over 1.3 mmX1.3 mm regions, considering a ratio of 100 between the diffusion coefficient in the PCW and that in cells lumen.

References

[1] Rohrbach & Luterbacher, Investigating the effects of substrate morphology and experimental conditions on the enzymatic hydrolysis of lignocellulosic biomass through modeling, *Biotechnology for Biofuels*, 14-103 (2021).

[2] M. Kfoury, et al., Upscaling fractured heterogeneous media: Permeability and mass exchange coefficient, *Journal of Applied Mechanics*, 73, 41-46 (2006).

[3] C. Loix et al., Reciprocal interactions between cadmium-induced cell wall responses and oxidative stress in plants, *Frontiers in Plant Science*, 8, 1867 (2017).

Linking Mineral Reactions with Induced Polarisation: A Microfluidic Study of FeS Formation and Dissolution

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Keywords: induced polarisation, iron sulphides, dissolution, microfluidics

Humans extract and disperse numerous substances from the subsurface, some of which are harmful to human health. Monitoring contamination—its movement, localization, and interaction with minerals—is critical for ensuring safety and guiding remediation efforts. Induced Polarisation (IP) is a valuable tool for observing underground flow and transport phenomena [1]. It is also sensitive to mineral processes such as nucleation, growth, dissolution, and passivation [2], which can result from interactions with contaminants [3]. However, in both column experiments and field studies (e.g., [4, 5]), it is challenging to accurately link specific mineral evolution to particular IP signals, as the minerals cannot be directly observed.

To address this, a series of microfluidic experiments will be performed to study precipitation and dissolution processes, with simultaneous acquisition of induced polarisation (IP) responses and in situ optical microscopy observations. Iron sulphides, specifically pyrite and mackinawite, are used in this study due to their pronounced IP response, high natural abundance, and critical role in governing contaminant mobility in subsurface environments [3]. The experimental investigation focuses on three fundamental geochemical processes: precipitation, dissolution, and passivation.

The first experimental phase focuses on pyrite precipitation, which requires anoxic conditions, at least one precursor, and an oxidising component [6]. Precipitation of mackinawite, a metastable precursor to pyrite, occurs under anoxic conditions and is comparatively more straightforward to achieve [7]. We expect an increase in IP signal with increasing surface area of precipitates. The second phase involves dissolving and/or passivating FeS. After attaching FeS to the microfluidic chip, an oxidising solution will be introduced to promote Fe^{2+} dissolution and the concurrent oxidation of both iron and sulphur, decreasing the IP signal with decreasing surface area. Alternatively, an iron oxide layer may form at the mineral surface, effectively passivating it and inhibiting further reaction.

In both experiments, we will measure the IP signal. We aim to correlate mineral evolution with the IP response, thereby improving the interpretation of IP data in field applications.

References

[1] Hermans, T. *et al.* Advancing measurements and representations of subsurface heterogeneity and dynamic processes: towards 4D hydrogeology. *Hydrology and Earth System Sciences* **27**, 255–287 (2023).
[2] Ntarlagiannis, D., Doherty, R. & Williams, K. H. Spectral induced polarization signatures of abiotic FeS precipitation. *GEOPHYSICS* **75**, F127–F133 (2010).
[3] Zhang, S. *et al.* Sulfidation of ferric (hydr)oxides and its implication on contaminants transformation: a review. *Science of The Total Environment* **816**, 151574 (2022).
[4] Slater, L., Ntarlagiannis, D., Personna, Y. R. & Hubbard, S. Pore-scale spectral induced polarization signatures associated with FeS biomineral transformations. *Geophysical Research Letters* **34**, (2007).
[5] Ciraula, D. A., Kleine-Marshall, B. I., Galeczka, I. M. & Lévy, L. Advanced Monitoring of H2S Injection through the Coupling of Reactive Transport Models and Geophysical Responses. *Environ. Sci. Technol.* **58**, 11128–11139 (2024).
[6] Benning, Liane G, Rick T Wilkin, and H. L Barnes, 'Reaction Pathways in the Fe–S System below 100°C'. *Chemical Geology* 167 (1): 25–51 (2000).
[7] Wolthers, M., Van der Gaast, S. J. & Rickard, D. The structure of disordered mackinawite. *American Mineralogist,* 88, 2007–2015 (2003).

From Anomalous Transport Of Red Blood Cells To O_2 Delivery In Vascular Networks

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Keywords: Biological Physics, Anomalous Transport, Blood Flow, Hypoxia

Microcirculation studies are starting to show the impact of transport in the brain vascular network on pathophysiology. For example, distributions of travel times, the times needed for blood to flow from one arteriolar end to a venular end, impacts the extraction of oxygen by tissue [1]. It has also been shown that anomalous transport arises from the vascular networks topology. A stochastic model of this behaviour identified fragile areas of the network, i.e. vessels that are only irrigated by long travel time pathways which bring insufficient amount of solute to surrounding tissues [2].

However, to isolate the impact that anomalous transport has on oxygen availability, oxygen confinement in red blood cells (RBC) and the oxygen-hemoglobin reaction were overlooked. In this work, we are expanding on the study of anomalous transport for oxygen in vascular networks by taking into account the bi-phasic nature of blood (plasma and RBCs), and the nonlinearity of the binding of oxygen to hemoglobin. We compute pressures, blood flow rates, and the ratio of RBC flow to blood flow (discharge hematocrit H_D) with a highly-resolved network simulation, which account for non-proportional distribution of RBCs at diverging bifurcations [3], in a mm^3 of mouse cortex. Based on these simulations and on theoretical arguments, we show that the distribution of transit times encountered by red blood cells is similar to that of solutes in blood (Fig. 1A). Moreover, the heterogeneity of hematocrit resulting from phase separation(Fig. 1B), induces a variability of oxygen concentration that is independent of travel times and increases the number of fragile vessels (Fig. 1C). Finally, we have seen that the non-linearity of oxygen binding impacts concentrations of oxygen in the plasma (Fig. 1C).

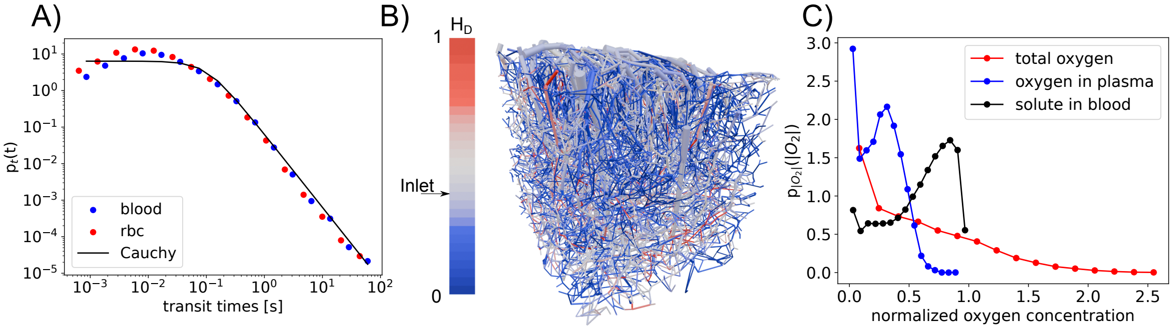

Figure 1: A) Probability density functions (PDF) of transit times (Blue: solute particles; Red: RBC; Dark line: approximate Cauchy distribution). B) Map of H_D in a microvascular network of mouse cortex, inlets at $H_D = 0.4$. C) PDF of oxygen normalized by the inlet values (Dark: for solute in monophasic fluid. Red: total oxygen in bi-phasic blood; Blue: oxygen in plasma).

References

[1] S. N. Jespersen and L. Ãstergaard. The roles of cerebral blood flow, capillary transit time heterogeneity, and oxygen tension in brain oxygenation and metabolism. *Journal of Cerebral Blood Flow & Metabolism*, 2012. doi: 10.1038/jcbfm.2011.153.

[2] F. Goirand, T. Le Borgne, and S. Lorthois. Network-driven anomalous transport is a fundamental component of brain microvascular dysfunction. *Nature Communications*, 2021. doi: 10.1038/s41467-021-27534-8.

[3] A. R. Pries, T. W. Secomb, P. Gaehtgens, and J. F. Gross. Blood flow in microvascular networks. Experiments and simulation. *Circulation research*, 1990. doi: 10.1161/01.res.67.4.826.

Modeling and Simulation of Ocean-Groundwater Interactions through the Beach: a Navier-Stokes and Richards Equations Coupling

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Keywords: Richards equation, Two-phase flows, Groundwater-ocean coupling

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The aim of this work is to reproduce accurately hydraulic interactions between oceanic waves and watersheds at a large space and time scales (from meters to kilometers and minutes to hours). This modeling is essential for accurate numerical simulations that can be used for regional forecasts in a context of climate change, particularly concerning water resources and morphodynamics issues. The problem of infiltration in the unsaturated zone, known as the vadose zone, appears to be the main obstacle to the relevance of predictions. Thus, it is at the core of the project, as infiltration, along with changes in the water table and streams, plays a key role in the hydraulic response of a watershed [2].

In this work, we propose a model to simulate the exchanges between the ocean and a groundwater table through the beach. To achieve this, a consistant coupling between surface flows (two-phase Navier-Stokes equations) and subsurface flows (mixed form of the Richards equation [3]) is proposed. It has been implemented in the massively parallel finite volume based code Notus (developed at the Institute of Mechanics and Engineering of Bordeaux), with particular attention given to the boundary conditions at the porous medium/surface interface to ensure mass and energy conservation during transfers, whether the porous medium receives mass (infiltration) or releases it (exfiltration).

Various strategies have been explored to achieve this coupling, including the use of the VANS model [1] to analyze the asymptotic models obtained on either side of the interface (Navier-Stokes for the exterior flow and Richards for the porous medium). Another possible approach involves applying a variable transformation to the Richards equation, facilitating the interaction between the two models.

After validation through several benchmark test cases from the literature [3, 4], the method was used to simulate the wetting of the La Verre dam and compared to results from [4].

References

[1] T. E. Geitani, S. Golshan, and B. Blais, ‘A high-order stabilized solver for the volume averaged Navier-Stokes equations’, Numerical Methods in Fluids, vol. 95, no. 6, pp. 1011–1033, Jun. 2023, doi: 10.1002/fld.5182.

[2] M. Ersoy, O. Lakkis, and P. Townsend, ‘A Saint-Venant Model for Overland Flows with Precipitation and Recharge’, Mathematical and Computational Applications, vol. 26, no. 1, Art. no. 1, Mar. 2021, doi: 10.3390/mca26010001.

[3] L. Orgogozo et al., ‘An open source massively parallel solver for Richards equation: Mechanistic modelling of water fluxes at the watershed scale’, Computer Physics Communications, vol. 185, no. 12, pp. 3358–3371, Dec. 2014, doi: 10.1016/j.cpc.2014.08.004..

[4] J.-B. Clément, ‘Numerical simulation of flows in unsaturated porous media by an adaptive discontinuous Galerkin method: application to sandy beaches’.

Flow and Phase Behavior of Nanoconfined Aqueous Solutions

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Keywords: Nanopores, aqueous solutions, flow dynamics, phase behavior

Aqueous solutions confined within nanopores and nanoporous materials are of fundamental importance in both natural and technological contexts. Nanoconfinement plays a critical role in biological processes such as water transport and ion regulation through cell aquaporins and ion channels. Beyond biology, confinement effects are central to a variety of applications, including water desalination, blue energy generation, energy storage, and the long-term durability of construction materials [1, 2, 3, 4].

The confinement within nanopores significantly alters the phase behavior, dynamics, and transport properties of liquids. For pure water, effects such as capillary condensation, freezing/melting shifts, glassy dynamics, and altered diffusion are well characterized [5, 6, 7]. In contrast, studies on aqueous solutions remain limited and often reveal unexpected phenomena due to spatial heterogeneity and interactions among the solvent, solute and pore walls, leading to nanophase separation and altered thermodynamic properties [8, 9]. These effects challenge classical thermodynamic models, particularly during phase transitions.

In this project, we aim to investigate the phase behavior and flow of aqueous solutions and the possible deviations from bulk behavior caused by confinement. Specifically, we focus on water condensation and evaporation in nanoporous silica with a pore size of 5 nm, in the presence of NaCl salt at varying concentrations. Solution activity and crystallization points are quantified using physisorption isotherms and optical methods. Concurrently, we employ molecular dynamics (MD) simulations to study the capillary flow of glycerol and ethylene glycol solutions within a single nanopore, with varying concentrations and interactions between the solvent, solute and pore walls.

Initial results from the MD simulations indicate that nanometric confinement significantly influences solution flow. Specifically, the solute exhibits a reduced filling rate and shows preferential adsorption at the pore walls relative to water, leading to partial demixing between the two components.

References

[1] Robertson, J.W.F., Engineered Nanopores for Bioanalytical Applications, Chap. 4. Elsevier, Amsterdam (2013)

[2] Cohen–Tanugi, D., Water desalination across nanoporous graphene, Nano Lett., 12(7), 3602–3608 (2012).

[3] Macha, M., 2D materials as an emerging platform for nanopore–based power generation, Nature Rev. Mater., 4(9), 588–605 (2019).

[4] Shao, H., Nanoporous carbon for electrochemical capacitive energy storage, Chem. Soc. Rev., 49(10), 3005–3039 (2020).

[5] Bergman, R., Dynamics of supercooled water in confined geometry, Nature, 403, 283–286 (2000)

[6] Jähnert, C., Melting and freezing of water in cylindrical silica nanopores, Phys. Chem. Chem. Phys., 10, 6039 (2008)

[7] Cerveny, J., Water dynamics in the hydration shells of biological and non-biological polymers, J. Chem. Phys., 150, 234904 (2019).

[8] Burba, C., Confinement Effects on the Phase Transition Temperature of Aqueous NaCl Solutions: The Extended Gibbs–Thomson Equation, Thermochim. Acta, 615, 81–87 (2015).

[9] Meissner, J., Secondary Confinement of Water Observed in Eutectic Melting of Aqueous Salt Systems in Nanopores, J. Phys. Chem. Lett., 7 (10), 1816–1820 (2016)

Synthesis and Characterization of Cage-like Mesoporous Silica SBA-16 to Study Cavitation in Confinement

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Keywords: Cage-like mesoporous silica, confinement, cavitation, nucleation

Cavitation, the formation of a vapor bubble in a metastable liquid, occurs in many situations ranging from engineering (ultrasonic cleaner, cavitation erosion) to natural science (embolism in trees). Bulk cavitation is qualitatively well described by the Classical Nucleation Theory (CNT), if the curvature dependence of the surface tension is taken into account [1,2]. On the other hand, in porous materials, cavitation is expected to depart from the bulk behaviour if it occurs in pores of size comparable to the critical bubble, in particular in porous materials with pores in the nanometre range and connected to the external gas reservoir through smaller apertures, as in mesoporous silicas with cage-like pores.

The first step consists in synthesising well-ordered mesoporous silica materials with large cage-like structure like SBA-16 [3]. The main geometric parameters relevant for cavitation are the radius of the spherical cages and the size of the windows connecting them, that can be varied thanks to different synthesis routes and/or post-synthesis treatments. The obtained mesoporous materials are then characterized using different techniques: sorption gas isotherms, Small-Angle X-ray Scattering (SAXS), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). Cross-analysis of the results is used to infer a clear picture of the porous material geometry, to be correlated with the cavitation experiments.

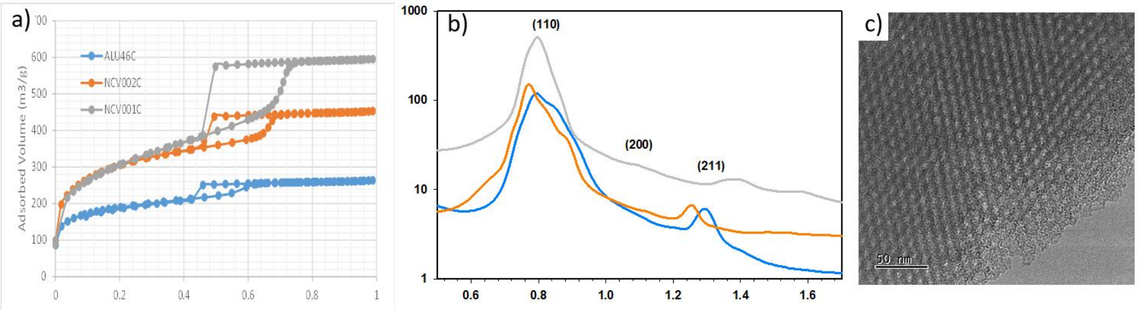

Figure: Illustration of SBA-16 characterization, using (a) gas sorption, (b) SAXS and (c) TEM.

References

[1] Doebele V., Benoit-Gonin A., Souris F., Cagnon L., Spathis P., Wolf P. E., Grosman A., Bossert M., Trimaille I., and Rolley E. Direct Observation of Homogeneous Cavitation in Nanopores. *Physical Review Letters* 125, 25, 255701 (2020).

[2] Bossert M., Grosman A., Trimaille I., Souris F., Doebele V., Benoit-Gonin A., Cagnon L., Spathis P., Wolf P.E., and Rolley E. Evaporation Process in Porous Silicon: Cavitation vs Pore Blocking. *Langmuir* 37, 49 14419–14428 (2021).

[3] Sakamoto, Y., Kaneda, M., Terasaki, O., Zhao, D. Y., Kim, J. M., Stucky, G., Shin, H. J., Ryoo, R. Direct Imaging of the Pores and Cages of Three-Dimensional Mesoporous Materials. *Nature* 408, 449-453 (2000).

A Novel Machine Learning-based Method for Groundwater Modelling involving Aquifer Rainfall Time Response Analysis and Clustering of Groundwater Wells

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Mots-Clés: eaux souterraines, apprentissage automatique, modélisation

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Multi-Physics Simulation of Void Evolution in Thermoset Prepreg UD Laminates

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Keywords: Porosity, Prepreg composite, Process simulation

Although porosity in thermoset prepregs is well controlled, faster manufacturing and new aerospace materials can trigger voids (e.g., through reduced autoclave pressure), compromising durability [1]. This study presents a numerical approach for predicting porosity by simulating the compaction and curing processes at the ply scale of thermoset UD laminates using OpenFOAM. The proposed modelling framework is divided into two phases: compaction and curing. During the compaction, an external pressure is applied to mimic the consolidation of the laminate stack. This phase captures the deformation of the ply and the corresponding resin redistribution within the interfibre spaces. The model resolves the evolution of the flow field within the porous network, thereby enabling a detailed assessment of the initial void content generated during compaction. In the curing phase, a key focus of the simulation is the variation of resin viscosity, which is affected by the local temperature field. The coupled thermo-mechanical simulation captures the interplay between heat generation, temperature evolution, and viscosity changes, ultimately affecting the closure or growth of voids, as seen in Figure 1.

Preliminary results indicate that both the applied compaction pressure and the viscosity profile are highly influential in determining the porosity level and bubble radius, according to literature [2,3]. Comparisons with experimental data from controlled synchrotron microtomography tests will be done to validate the effectiveness of the modelling approach. A 4D in-situ compaction and curing test will be achieved, with two different resolutions: one to see interfibre voids and the other one at a mesoscale resolution. In conclusion, this study establishes a robust simulation framework for predicting porosity in thermoset resin prepreg UD laminates. Future work will extend the model to incorporate additional factors such as diffusion mechanisms, layer stacking sequence, and the homogenisation from microscale in OpenFOAM to macroscale in the finite element software Abaqus, with the aim of a manufacturing process simulation at the part scale.

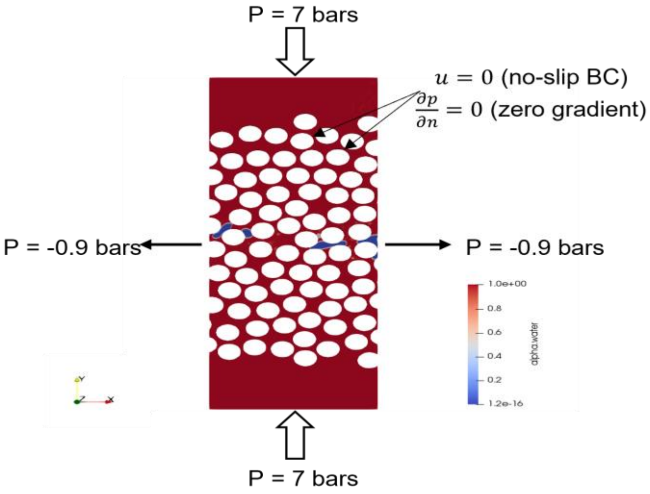

Figure 1: Remaining voids during curing and applied boundary conditions.

References

[1] Elnekhaily, S. A., Effects of micro voids on the early stage of transverse crack formation in unidirectional composites. *Composites Part A: Applied Science and Manufacturing*, *167*, 107457, (2023).

[2] Mehdikhani, M., Voids in fiber-reinforced polymer composites: A review on their formation, characteristics, and effects on mechanical performance. *Journal of Composite Materials*, *53*(12), 1579–1669 (2018).

[3] Agius, S. L., Cure behaviour and void development within rapidly cured out-of-autoclave composites. *Composites Part B: Engineering*, *47*, 230–237 (2013).

Controls Of Double-Porosity Interconnectivity On Dissolution Of Carbonate Rocks

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Keywords: Carbonate rocks, dissolution, reactive transport, double-porosity, interconnectivity

Carbonate rocks are widespread and highly reactive, making their study a key topic for various environmental and anthropogenic issues. Dissolution of carbonate rocks is controlled by different factors, related to the fluid (chemical composition, pH, flow velocity) or the rock (mineral content, porosity, permeability, microstructure), and results in different dissolution patterns. Even though microstructural controls on dissolution processes have been previously evidenced, the specific contribution of the double porosity (i.e., the intergranular macroporosity and intragranular microporosity) remains unclear, and is so far poorly considered in experimental and numerical studies. To investigate the specific impact of the double-porosity interconnectivity on the dissolution of carbonate rocks, we perform controlled dissolution experiments under identical experimental conditions on two nearly pure calcite limestones (Euville and Lavoux) characterized by different grain and pore structures. Two flow rates are applied to investigate the effect of various hydrodynamic conditions. At high flow rates, two distinct dissolution patterns are evidenced: for Euville samples, dissolution is distributed across the entire width of the sample, whereas for Lavoux samples, dissolution is localized in wormhole-type channels. At lower flow rates, similar wormhole-type dissolution patterns are observed for both Euville and Lavoux samples. We explain these contrasting responses by differences in pore interconnectivity, resulting in different accessible specific surface areas and reactivity. Specific expressions of Péclet and Damköhler numbers accounting for the intrinsic accessibility to the intragranular microporosity and the associated specific surface area are used and allow the two limestones to be clearly positioned in areas of *Pe-Da* diagram consistent with the observed dissolution patterns. Finally, numerical transport modeling approach using Lattice-Boltzmann Method is proposed to support our hypotheses.

~~Pore-scale modeling of diffusiophoresis for groundwater remediation~~

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Keywords: Diffusiophoresis, Particle transport, Concentration gradient, OpenFOAM simulations

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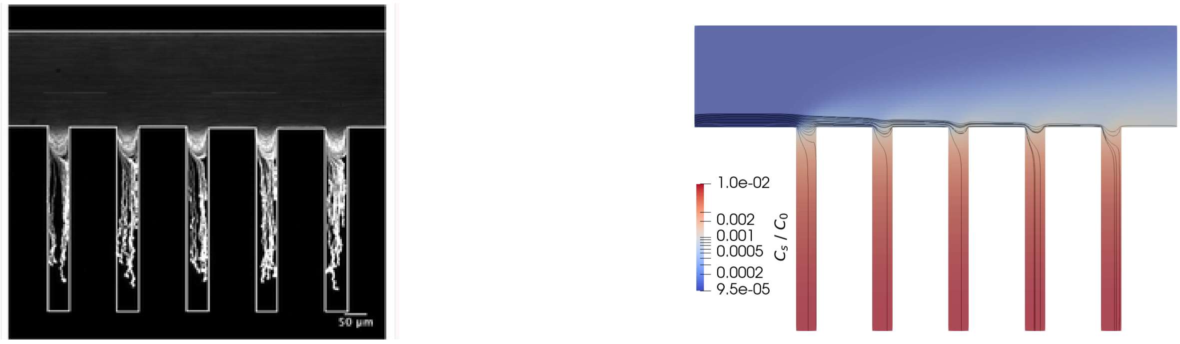
The presence of pollutants in soils and geological formations poses a serious threat to groundwater quality, often resulting in long-term contamination of water resources. Even after remediation, residual contaminants can remain trapped by capillary forces, slowly releasing toxic compounds with time. These pollutants are among the most difficult to remove from porous media. Promising remediation approaches involve colloidal particles – such as bacteria or nanoparticles. However, a major challenge is the efficient transport of these colloids to contaminated zones, which are often isolated from the main flow paths. Diffusiophoresis is a transport mechanism that drives colloids along concentration gradients [3]. We investigate the possibility that pollutant-induced concentration gradients can actively guide particles toward contaminated regions. However, an effective theory including diffusiophoresis in models of particle transport in porous media is still lacking. There is currently no suitable model for diffusiophoresis in porous media. One challenge lies in accurately representing the concentration gradient and boundary conditions for porous media, particularly the interactions between the porous matrix and the particles.

In this study, we develop an OpenFOAM-based pore-scale simulator to model the transport of colloidal particles driven by diffusiophoresis. The diffusiophoretic velocity – which accounts for both electrophoretic and chemiphoretic contributions [4, 6] – is incorporated into an advection-diffusion framework [1] to capture the influence of solute concentration gradients on particle motion. We conducted pore-scale simulations in OpenFOAM to analyze the evolution of solute gradients and resulting particle trajectories within porous structures. The simulation results are compared with experimental observations from the literature (e.g., main channels with dead-end pores [2], Figure 1) and with ongoing microfluidic experiments [5]. This work advances the understanding of diffusiophoresis in porous media and marks a step forward in modeling its potential role in environmental remediation.



(a) (b)

Figure 1: Particle trajectory capture in dead-end pores via diffusiophoresis: (a) Experimental data from Battat et al. [2] and (b) OpenFOAM simulation with solute concentration gradients displayed on a logarithmic color scale.

References

[1] Ault, J. T., Shin, S., and Stone, H. A. (2018). Diffusiophoresis in narrow channel flows. *Journal of Fluid Mechanics*, 854:420–448.

[2] Battat, S., Ault, J. T., Shin, S., Khodaparast, S., and Stone, H. A. (2019). Particle entrainment in dead-end pores by diffusiophoresis. *Soft Matter*, 15(19):3879–3885. Publisher: The Royal Society of Chemistry.

[3] Derjaguin, B. V., Sidorenkov, G., Zubashchenko, E., and Kiseleva, E. (1947). Kinetic Phenomena in the boundary layers of liquids 1. the capillary osmosis. *Progress in Surface Science*, 43(1):138–152.

[4] Prieve, D. C., Anderson, J. L., Ebel, J. P., and Lowell, M. E. (1984). Motion of a particle generated by chemical gradients. Part 2. Electrolytes. *Journal of Fluid Mechanics*, 148:247–269.

[5] Roman, S. and Rembert, F. (2025). Inhibition of mineral dissolution by aggregation of colloidal particles driven by diffusiophoresis. *Physical Review Fluids*, 10(3):L032501. Publisher: American Physical Society.

[6] Velegol, D., Garg, A., Guha, R., Kar, A., and Kumar, M. (2016). Origins of concentration gradients for diffusiophoresis. *Soft Matter*, 12(21):4686–4703.

Characterization of the porous network and particle density under compression using XCT of a bio-based porous media

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Keywords: Bio-based porous media, PNM, image analysis

This study focuses on analyzing the microstructural evolution of hemp shiv particules, a sustainable bio-based building material, under varying compression states. When used in insulation systems, such materials contribute to carbon neutrality by reducing CO_2 emissions. Therefore, understanding the relationship between their microstructure and multiphysical behavior is crucial for optimizing these systems.

X-ray tomography was conducted at the Soleil Synchrotron (Anatomix beamline) on cylindrical samples (40 mm in diameter and height), scanned in both loose and compressed states (densities ranging from 130 to 844 kg/m³). In addition to traditional reconstruction, the Paganin filter [1] was applied to enhance image contrast, although challenges remained due to high intra- and inter-particle porosity, complex particle morphology, imaging artifacts, and large data volume. To address these challenges, deep learning was employed using a U-Net convolutional neural network implemented in Dragonfly software [2], combined with a watershed algorithm to segment and separate over 2,000 individual hemp shiv particles. Then, morphological analysis including Feret diameter distribution and shape characterization through inertia tensor approximation were conducted.

Furthermore, local particle density was estimated by correlating X-ray grey values with calibration data from materials of known densities [3], assuming a linear relationship between attenuation and density. These values were validated experimentally using solid pycnometry [4].

In addition, the segmented pore space was converted into digital pore networks using PoreSpy and OpenPNM [5], enabling analysis of pore size distribution, connectivity, permeability, and tortuosity as a function of compression.

Overall, this work highlights the effectiveness of combining synchrotron X-ray tomography with advanced image analysis techniques for characterizing complex porous bio-based materials, offering methodologies applicable to a wide range of materials with challenging geometries and imaging conditions.

References

[1] Paganin, D., Mayo, S. C., Gureyev, T. E., Miller, P. R. and Wilkins, S. W, Simultaneous phase and amplitude extraction from a single defocused image of a homogeneous object. Journal of Microscopy, 206: 33-40 (2002).

[2] Dragonfly 2022.2 [Computer software]. Comet Technologies Canada Inc., Montreal, Canada; software available at https://www.theobjects.com/dragonfly.

[3] P. Glé, T. Lecompte, A. Hellouin de Ménibus, H. Lenormand, S. Arufe, C. Chateau, V. Fierro, A. Celzard: Densities of hemp shiv for building: From multiscale characterisation to application, Industrial Crops and Products, vol. 164, p. 113390 (2021).

[4] H. Ratsimbazafy. Évaluation du potentiel de co-produits agricoles locaux valorisables dans le domaine des matériaux de construction (PALOMAC). Matériaux. Université Paul Sabatier - Toulouse III (2022).

[5] J. Gostick, M. Aghighi, J. Hinebaugh, T. Tranter, M. A. Hoeh, H. Day, B. Spellacy, M. H. Sharqawy, A. Bazylak, A. Burns, W. Lehnert, and A. Putz: OpenPNM: A Pore Network Modeling Package, Computing in Science and Engineering, vol. 18, p. 60–74 (2016).

Probing Particle Dynamics Inside Opaque Porous Media Using X-ray Radiography

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Keywords: diffusion, sedimentation, x-rays

Typically, experiments measuring colloid transport in porous media use optically transparent, indexed-matched media, in order to be able to resolve the dynamics of the colloids with optical microscopy. However, naturally occurring porous media, such as soils are opaque. We use X-ray radiography to probe colloid transport inside opaque porous media. We analyse our data in the reciprocal space using X-ray Dynamic Differential Radiography (XDDR) [1], the X-ray equivalent of Dynamic Differential Microscopy (DDM) [2]. We also carry out simulations of colloid transport in a porous medium, which include hydrodynamic interactions, and compare.

References

[1] P. Levitz et al. “Probing particle dynamics in a fully opaque porous network using X-ray differential dynamic radiography (XDDR)”, *Soft Matter*, 10.1039 (2025).
[2] Fabio Giavazzi et al. “Scattering information obtained by optical microscopy: Differential dynamic microscopy and beyond”, *Phys. Rev. E*, 80.3, p. 031403 (2009).
[3] Author6, *Book title*, page numbers. Publisher, place (year).

Mesofauna Activity and Soil Pore Space Dynamics: Temporal Analysis Using X-ray Microtomography

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Keywords: Soil, X-ray tomography, Bioturbation

Mediterranean agroecosystems, which account for a substantial portion of European horticultural production, are particularly vulnerable to the effects of climate change. This vulnerability is exacerbated by soil degradation, rising temperatures, and the increased frequency of extreme weather events. To ensure a successful agroecological transition in these regions, it is crucial to preserve the ecosystem services provided by soils. Soil fauna plays a key role in the exchanges between atmosphere and pedosphere through the edaphic fauna activity, thereby influencing the transfer of mass and energy within the soil, a porous and dynamic medium.

This study focuses on the impact of bioturbation activities of enchytraeids on the structure of soil pore space. Enchytraeids are Annelida Oligochaeta that measure between 100 and 2000 µm in diameter and 6 to 50 mm in length. They are ubiquitous in soils and present in various ecosystems [1]. Recognized as model organisms for their role in decomposing organic matter [2] and as bioindicators of soil health [3], their bioturbation activity creates a network of galleries that remains understudied to date [4]. Yet, a recent experimental study [5] has demonstrated that enchytraeids modify the pore space configuration and shift the pore size distribution around their diameter.

An ongoing experiment is set to observe the evolution of this pore space under the influence of enchytraeid bioturbation. This study aims to examine changes in the morphological and hydraulic properties of soil over time, using experimental mesocosms observed via X-ray microtomography. Three experimental conditions are being tested: (i) the presence of 60 individuals (30 *E. bulbosus*, 30 *E. lacteus*), representing a typical density of representative species in Mediterranean soils, (ii) 10 individuals (5 *E. bulbosus*, 5 *E. lacteus*), and (iii) no enchytraeids (control). The samples are then subjected to water transfer in a specially developed experimental rain simulator.

The results highlight the importance of considering the modifications of pore space induced by soil mesofauna, a factor currently overlooked in models of energy and mass transfer at the soil profile scale.

[1] Orgiazzi A. et al., Global Soil Biodiversity Atlas. European Commission, Publications Office of the European Union,176 pp (2016)
[2] Cole, L. et al., Enchytraeid worm (Oligochaeta) influences on microbial community structure, nutrient dynamics and plant growth in blanket peat subjected to warming. Soil Biology & Biochemistry, 34, 83-92 (2002)
[3] Pelosi, C. et al., Enchytraeids as bioindicators of land use and management, Applied Soil Ecology, 123, 775-779 (2018)
[4] Porre, R. J. et al., Exploring the relationship between soil mesofauna, soil structure and N2O emissions, Soil Biology and Biochemistry, 96, 55-64 (2016)
[5] Serbource, C. et al., Enchytreids : Small buy important ecosystem engineers, Geoderma, 453, 117-150 (2025)

Morphology probed locally through tortuosimetric analysis

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Keywords: Microstructure, Morphology, Connectivity, Local Features, Geodesic Distance Transform, Tortuosity

Porous material numerical characterisation is of paramount interest in a wide range of applications. The extraction of reliable and relevant features that accurately describe the complex morphology of materials, is a delicate task. Tortuosity [1], a multifaceted concept, is one of the key characteristics of material, in the broadest sense of the term. The tortuosity τ under consideration in this study is defined by the ratio of the geodesic distance D_G by the Euclidean distance D_E:

$$\tau = \frac{D_G}{D_E}, \tag{1}$$

yielding a morphological depiction of microstructures [2]. By leveraging the versatility of geodesic distance transform to consider gray-level images, we propose an extension of the original *M-tortuosity* which allows the analysis of non-segmented images of real materials and of binary microstructures enhanced by local feature maps. The efficiency of the *M-tortuosity* is demonstrated through its application on Boolean schemes that simulate heterogeneous complex microstructures (see Fig. 1). This innovative solution is made accessible through an easy-to-use plug-in in a free-access software named *plug im!*.

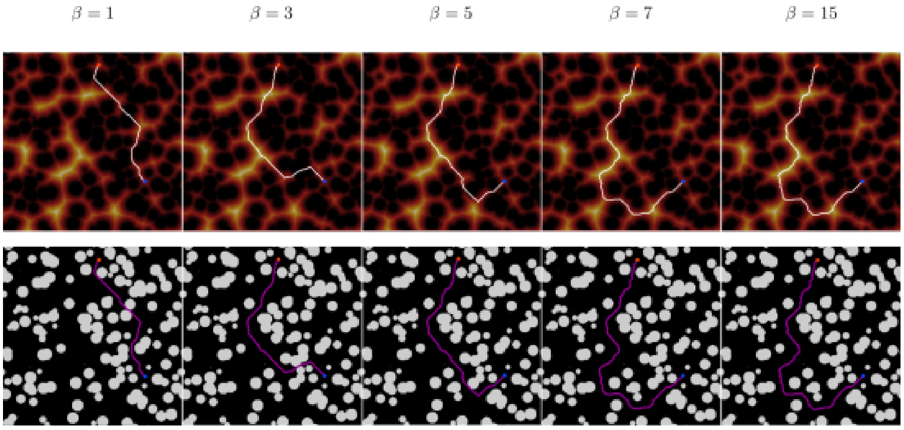

Figure 1: **Narrowness Enhanced Morphology**: Evolution of the geodesic path (white and purple curves) between two arbitrary points (blue and orange dots) according to the sensitivity β to the local narrowness. The microstructure (bottom row) is enhanced by its local narrowness map (top row). The geodesic path, originally the shortest between blue and orange dots ($\beta = 1$), increases with β until convergence is reached ($\beta = 7$).

References

[1] Clennell, M. B., Tortuosity: a guide through the maze, Geological Society, London, Special Publications, 122(1), 299-344 (1997)

[2] Chaniot, J., Moreaud, M., Sorbier, L., Marquet, P., Becker, J. M., & Fournel, T., Characterizing microstructures with representative tortuosities, Science and Technology for Energy Transition, 79, 31, (2024)

Elastic Properties of Partially Saturated Tournemire Shale at Seismic Frequencies

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Keywords: Shale, Attenuation, Seismic monitoring

Understanding the impact of hydraulic loads on fault zones in shale formations is critical to safely storing nuclear waste in such formations. The CHENILLE project performed fluid injection experiments in a fault zone in the Tournemire/France underground research lab (URL) and monitored the experiments with a system of acoustic emissions (AE) and broad band seismic sensors [1]. The analysis is challenging because of the transverse isotropy (TI) of the elastic properties of the shale and due to the frequency dependence of the stiffness components at elevated water content. To complement the field experiments, we performed laboratory measurements on core samples taken from the URL to investigate the dispersion of elastic properties and intrinsic attenuation at seismic frequencies.

The stress-strain response of samples was measured during the application of axial sinusoidal oscillations in the seismic frequency range (0.1 – 1000 Hz). With strains of $<10^{-5}$ the measurements are in the linear elastic regime. Frequency dependent Young's moduli were determined on three Tournemire shale samples with bedding orientations of 0°, 45° and 90°. Poisson's ratios were determined on the 0° and 90° samples. From these we calculate the five stiffness components of TI anisotropy. Additionally, we measured the P-wave velocities at ultrasonic frequencies. Initial measurements were performed on samples taken directly from the vacuum packaging, with the assumption that the water saturation is equivalent to that of the formation of 90% [2]. Following the first round of experiments, the samples were placed in a vacuum chamber with a potassium sulphate solution to maintain a relative humidity of 98-97% [3].

The elastic properties of Tournemire shale exhibit dispersion at seismic frequencies. The dispersion is accompanied by significant intrinsic attenuation, with a maximum at 100-200 Hz, which is in the frequency range of the seismic surveys conducted during the Chenille project. These measurements confirm previously observed dispersion in wave velocities between ultrasonic and seismic frequencies [4]. Following the increase in water saturation, we observe a decrease of the elastic moduli and an increase of the intrinsic attenuation. Accounting for the viscoelastic response of the shale in the initial velocity models could improve the 3D seismic tomographic inversion as well as the AE location estimation.

References

[1] Bonnelye et al., CHENILLE: Coupled Behavior Understanding of Faults: from the Laboratory to the Field, *Advances in Geosciences,* 58, 177–188 (2023).
[2] Valès et al., Experimental study of the influence of the degree of saturation on physical and mechanical properties in Tournemire shale (France), *Applied Clay Science*, 26 (1-4), 197-207 (2004).
[3] Greenspan, Humiditz Fixed Points of Binarz Saturated Aqueous Solutions, *Journal of Research of the National Bureau of Standards – A. Physics and Chemistry,* 81, 89-96 (1976).
[4] Zillmer et al., In situ seismic measurements in claystone at Tournemire (France), *Geophysical Journal International*, 199, 1798-1807 (2014).

Implementing Contact-Mechanics In Faulted Porous Media Using VEM

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Keywords: contact-mechanics, polyhedric meshes, Virtual Element Method (VEM)

Thermo-Hydro-Mechanical models in faulted porous media play an important role in many applications in geosciences. Fault networks act as corridors for fluid flows and associated mass and energy transfers and they have a preeminent role on stress (re)distribution interacting with these transfers. Numerical modelling is a key tool to better understand, assess and control these processes. They couple the flow and energy transport along the faults and in the surrounding porous rock, the rock mechanical deformation, and the mechanical behavior of the faults related to contact-mechanics [1].

The ComPASS project (https://gitlab.com/compass) aims to provide a generic, open-source, user-friendly platform to conduct high-performance simulations of multicomponent multiphase non-isothermal flows in faulted porous media. The main objective is to create a quantitative subsurface model to better understand phenomenon such as fault reactivation, with applications in geoscience fields like geothermy, CO2 underground storage, etc. [2, 3]. It is developed in collaboration between the French National Geological Service (BRGM), the University Côte d'Azur (UniCA) and the French National Agency for radioactive waste management (ANDRA).

In this talk, we will focus on the simulation of contact-mechanics in a faulted porous medium. First, we will present a discretization of the elastic deformation problem using the Virtual Element Method (VEM), which is a natural extension of the P1 Finite Element Method (FEM) to polyhedral meshes. Then we will discuss the implementation of Coulomb-type contact mechanics across faults, using face-wise constant unknowns for contact surface tractions at the matrix-fault interfaces. This choice allows to cope with fault networks including corners, tips and intersections and leads to contact conditions local to each fault face, that can be solved with efficient semi-smooth Newton non-linear solvers. Its requires a stabilisation which is achieved by enrichment of the displacement field with an additional "virtual" bubble unknown at one side of each fault face [4]. Lastly, we will consider the fully coupled thermo-hydro-mechanical problem. Because this problem results in a very large and usually badly conditioned linear system, we will address it through a possibly accelerated iterative coupling algorithm.

This post-doctoral project is part of the ANR PRCE EARTH-BEAT 2024-2028 "Transient Thermo-Hydro-Mechanical couplings in hydrothermal systems – application to geothermal energy and giant mineral resources" (funded by the French National Research Agency under grant number ANR-23-CE50-0027).

References

[1] F. Bonaldi, J. Droniou, R. Masson, A. Pasteau, Energy stable discretization of two-phase flow in deformable porous media with frictional contact at matrix-fracture interfaces, Journal of Computational Physics, 455 (2022)

[2] F. Xing, R. Masson, S. Lopez, Parallel numerical modeling of hybrid-dimensional compositional non-isothermal Darcy flows in fractured porous media, Journal of Computational Physics, 345, 637–664 (2017)

[3] A. Armandine Les Landes, L. Beaude, D. Castanon Quiroz, L. Jeannin, S. Lopez, F. Smaï, T. Guillon, R. Masson, Geothermal Modeling in Complex Geological Systems with ComPASS, preprint (2023)

[4] J. Droniou, G. Enchéry, A. Haidar, I. Faille, A. Haidar, R. Masson, A bubble VEM-fully discrete polytopal scheme for mixed-dimensional poromechanics with frictional contact at matrix-fracture interfaces, Computer Methods in Applied Mechanics and Engineering, 422, 116838 (2024)

Euler-Euler Simulations Of Colloidal Transport And Retention At The Pore Scale

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Keywords: Euler-Euler simulation, Clogging, NAPL

Non-aqueous liquids (NAPLs) are water-immiscible pollutants that can disperse and release significant amounts of toxic compounds into underground water resources. Numerous methods have been developed to remove these pollutants from aquifers, but NAPL droplets remain trapped by capillary forces in the porous matrix even after depollution. The aim of our research is to explore the potential of colloids (e.g. nanoparticles, bacteria) to remobilize immiscible pollutant droplets. Our final objective is to develop a multiphase model at the pore scale that includes colloidal interactions with the solid phase, the aqueous phase, and the NAPL. Euler-Lagrange models allow an accurate description of colloidal particle interactions (e.g. transport and retention) but remains very time- and resource-intensive. In this work, we are developing Euler-Euler approaches based on OpenFOAM's multiphaseEuler module to represent particles as a dispersed phase in water. The use of this model in the context of the remediation of polluted porous media is currently under development. Our package includes new viscosity models and plastic behavior, as well as poromechanic properties to account for the compressibility threshold of clogged particles. Aggregation forces in between particles and between particles and grains are also considered. To this end, we are using DLVO theory, which characterizes the forces exerted between two charged surfaces separated by a liquid. We present preliminary results such as : i) comparisons with Euler-Lagrange simulations for very diluted suspension, ii) response to fluid stresses and its compressibility, and iii) study of the impact of particle aggregation in the context of porous media.

Averaging random conduit networks, influence of conductivity randomness

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Keywords: Random Networks, Percolation, Averaging

Karst aquifers and fractured porous media are natural examples of complex conduit networks, where flow is controlled by both the geometry of the network and the disorder in local conductivities [2]. Accurately predicting flow through such systems requires models that capture both the structural complexity and the disorder of hydraulic properties.

In this study, we investigate how conductivity disorder influences the effective hydraulic properties of random conduit networks. By combining perturbation theory, mean-field approximations, and power-averaging techniques [1], we derive expressions that describe how both network connectivity and conductivity disorder control the large-scale flow behavior.

A key result is the derivation of an effective power-law averaging formula, where the exponent is linked to the product of the local conductivity and the associated resistance distance. Notably, the averaged exponent depends only on the network geometry and remains stable regardless of the conductivity variance, supporting the robustness of the approach across a broad range of heterogeneity.

Numerical simulations on synthetic 2D and 3D networks support the theoretical developments and illustrate the robustness of the approach, even at high levels of disorder. These insights contribute to the development of upscaling methods for complex subsurface flow systems, with potential applications to karst aquifers and other heterogeneous networks.

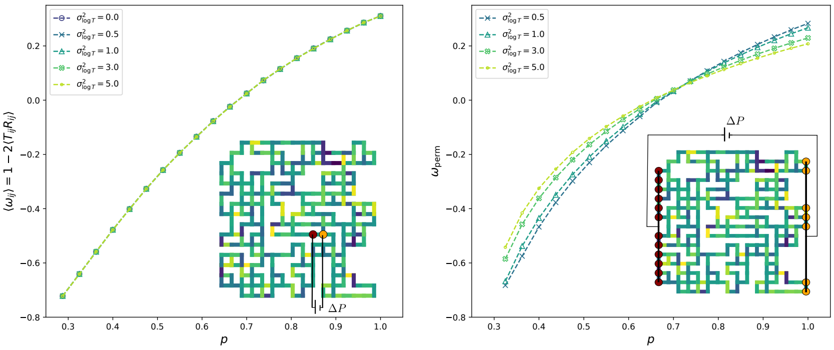

Figure 1: Power averaging exponent ω as a function of the percolation parameter p, the probability of retaining an edge, in a 3D percolation network ($64 \times 64 \times 64$ nodes). **Left:** ω computed as $1 - 2\langle R_{ij} T_{ij} \rangle$, where R_{ij} is the resistance distance between adjacent nodes and T_{ij} is the edge conductance, averaged over all edges. **Right:** ω estimated from flow simulations using permeameter boundary conditions. Both approaches yield consistent estimates of ω. In particular, the first definition shows that ω depends only on the network topology and remains independent of the conductivity distribution.

This work was funded by ERC grant #101071836.

References

[1] Colecchio I., Le Gall E., Noetinger B., Effective conductivity of conduit networks with random conductivities, *arXiv:2503.09457* [cond-mat.dis-nn] (2025). `https://arxiv.org/abs/2503.09457`

[2] Collon P., Bernasconi D., Vuilleumier C., Renard P., Statistical metrics for the characterization of karst network geometry and topology, *Geomorphology*, **283**, 122–142 (2017).

Predicting Seismic Response To Fluid Injection Using Machine Learning

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Keywords: Induced seismicity, Machine learning, Numerical method

Seismicity induced by fluid injection (*e.g.* enhanced geothermal systems, CO_2 storage, wastewater injection) remains a significant concern of risk for communities and industry as it may cause structural damages and economic losses. While it is crucial to anticipate and control this risk, understanding the relation between fluid injection and seismicity represents a real challenge, as it depends on multiple complex parameters like the geological characteristics of the environment, medium porosity, faults locations, or the reservoir geometry. In this work, we present an innovative machine learning approach designed to 1/ capture the relation between fluid injection and seismicity and 2/ use it to forecast the future number of earthquakes on a fixed time scale of interest. Our model is distinguished by its relative simplicity, as it relies on a linear regression between the seismicity rate and the injected volume time series. Consequently, our approach does not require advanced knowledge of complex physical parameters that may be unknown or poorly constrained, allowing our model to be used in a wide range of applications. Moreover, our strategy also allows us to overcome the difficulty posed by the important time lag between the injection variations and the associated seismic response (controlled in particular by the hydraulic diffusion rate in a porous medium). We apply our method to the significant rise of the seismicity in Oklahoma (United States), caused by massive injections of waste water into the ground since 2010. By training our model to capture the injection/seismicity relation during several years, we could forecast the number of future induced earthquakes, as shown in Fig 1. This work opens up a wide range of new application prospects, such as its application to fluid-induced seismicity during geothermal operations or CO_2 storage.

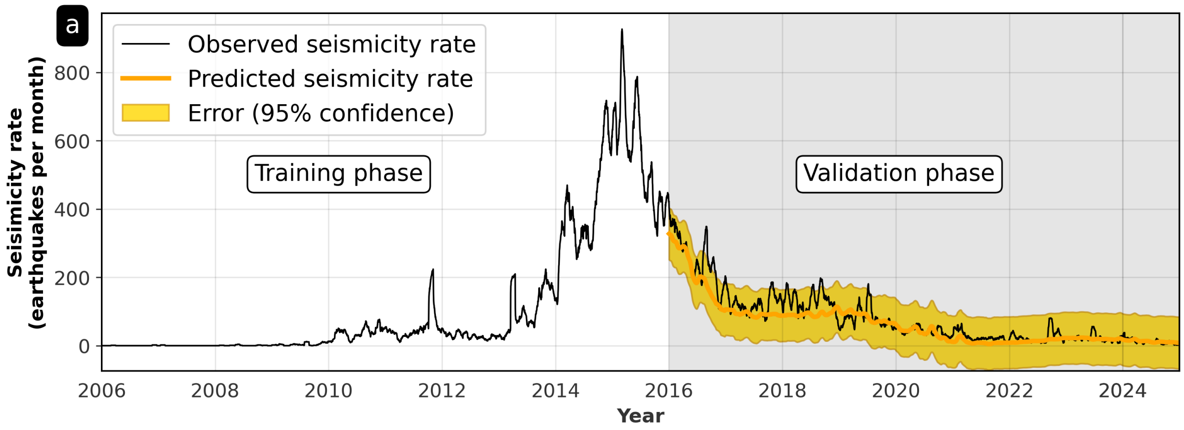

Figure 1: Prediction of the induced seismicity in Oklahoma (United States).

Tuning Wettability of Microfluidic Devices via *In Situ* Plasma Treatment

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Keywords: microfluidics, porous media, plasma treatment

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.

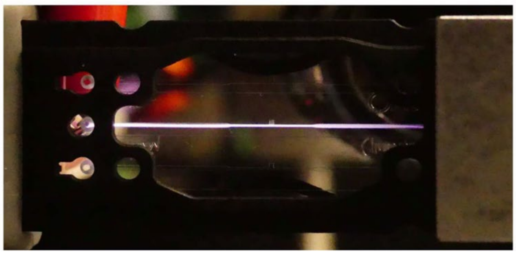

Figure 1: Picture of glass microfluidic device during plasma treatment. [1]

This study demonstrates the successful generation and propagation of atmospheric pressure helium plasma within sealed glass microfluidic devices for *in situ* wettability treatment. A 1 minute plasma exposure significantly increased surface hydrophilicity, confirmed by contact angle measurements. Wettability stability was investigated under air and water storage, with water extending hydrophilic effects for up to 70 days. X-ray photoelectron spectroscopy revealed cleaning and surface functionalization as key mechanisms. The setup allows treatment of internal microchannel surfaces and enables selective plasma targeting via electrode placement.

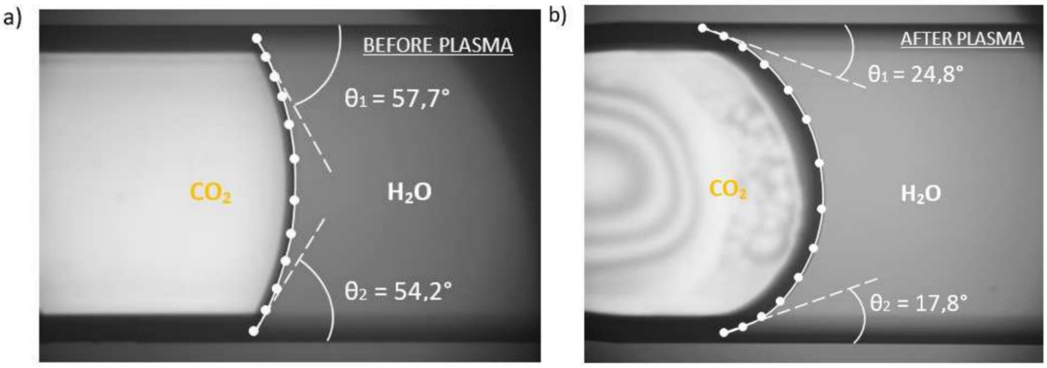

Figure 2 : CO_2-water interface before plasma treatment (a) after 1 min plasma treatment (b) [1].

References

[1] V. Gredicak et al, Microfluids and Nanofluidics, 29 (4), 22 (2025)

Assessment of grid resolution for using Poisson-Nernst-Planck equations in reactive transport modeling.

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Christophe Tournassat

Philippe Leroy

Reactive transport models combine transport and chemical reactivity equations to simulate mass transfers in porous media. Because it is not feasible to include all the terms to be used for a complete description of a geological system, primary variables must be selected according to the problem being addressed, and so some approximations or simplifications must be made. Consequently, the range of conditions in which these simplifications remain valid must be estimated. In this work, we focus on the electrical voltage, especially concerning ion diffusion currents created by the difference in ion mobility in aqueous phases. In the absence of an applied external electrical potential gradient, self-induced electrical potential differences slow down the ions with the greatest diffusion coefficient and accelerate the slowest ions. This phenomenon is the conjugate effect of electromigration, which consists of the forced diffusion of ions exposed to an applied gradient of electrical potential. Diffusion currents and electromigration have attracted a great deal of attention from scientists in various fields with applications in advanced electronics, neurobiology, and Earth sciences, e.g., to model junction and membrane potentials. Electromigration can be described by the Nernst-Planck equations and the conservation of mass equation (continuity equation). In reactive transport modelling studies, a local electroneutrality condition is often assumed instead of solving the full Poisson-Nernst-Planck equation. The local electroneutrality condition reduces the number of primary variables to be solved, and the related approximation is justified by the accuracy of the numerical algorithms used to solve the transport equations at the resolution scale of reactive transport models. However, as the considered resolution is increased, the resolution of the full Poisson-Nernst-Planck equations becomes necessary. This work intends to quantify the quality of the reactive transport predictions using the electroneutrality condition as a function of grid resolution by comparing results with those obtained with the Poisson-Nernst-Planck equations.

A Physical Approach to the Modeling of Hygrothermal Transfers in Bio-Based Building Materials

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Keywords: Bio-based materials, Hygrothermal transfers, Macroscopic Modeling, Porous Media

Bio-based building materials are increasingly recognized as a promising solution to reduce carbon emissions associated with the construction sector. Beyond their renewable origin, they exhibit the ability to buffer temperature and humidity fluctuations when used as insulation materials. Despite these advantages, their integration into conventional energy models remains challenging due to the strong coupling between heat and moisture transport phenomena, as well as the diversity of their physical properties.

Classical models often fail to accurately predict these transfers, as they rely on phenomenological approaches and introduce effective coefficients that lack physical meaning [1]. In particular, bound water transport, referring to water absorbed by fibers, is poorly understood, sometimes neglected, or merged into a global moisture transfer that also includes vapor. However, recent studies have shown that bound water flux can dominate over vapor flux under certain conditions. Moreover, Zou et al. have characterized the diffusion coefficients of bound water and vapor using an innovative NMR and MRI technique [2]. They also proposed a moisture model that distinguishes between the two transport mechanisms [3], yielding predictions that closely match experimental observations. By extending this model to non-isothermal conditions, the present work aims to develop a macroscopic model of hygrothermal transfer based on a local description that explicitly accounts for both vapor and bound water transport.

The hygrothermal model consists of two coupled partial differential equations, whose main potentials are relative humidity ϕ and temperature T. Both equations exhibit a symmetrical structure. Scaling the model allows for the definition of fundamental dimensionless numbers which govern the hygrothermal behavior of the bio-based material:

$$L = \frac{h_{bv}}{\Delta T_0 c_{p,b}}, \quad H_t = \frac{\lambda_0}{D_{b_0}(1-\varepsilon)\rho_s c_{p,b}}, \quad H_y = \frac{\varepsilon D_v \rho_0}{(1-\varepsilon)\rho_s D_{b_0}}. \tag{1}$$

In the first number, h_{bv} denotes the latent heat of water evaporation, ΔT_0 is a characteristic temperature difference and $c_{p,b}$ is the specific heat capacity of bound water. In the hygrothermal number H_t appear a characteristic thermal conductivity λ_0, the material's porosity ε and dry solid density ρ_s, as well as the reference bound water diffusion coefficient D_{b_0}. In the hygroscopic number H_y, the vapor diffusion coefficient is D_v and the characteristic vapor saturation density is ρ_0.

Based on typical literature values under ambient conditions for the characteristic physical properties, the orders of magnitude of these numbers are estimated as follows:

$$L \sim 20, \quad H_t \sim 300, \quad H_y \sim 1. \tag{2}$$

Consequently, the computations suggest that heat transfer dynamics are significantly faster than moisture transport. The dimensionless numbers can also provide valuable insights into the different coupling regimes and the dominant transport mechanisms.

References

[1] Kunzel, Simultaneous Heat and Moisture Transport in Building Components: One-and two-dimensional calculation, (1995)

[2] Zou et al., Fast transport diffusion of bound water in cellulose fiber network, Cellulose, vol. 30, pp 7463-7478 (2023)

[3] Zou et al., Unveiling moisture transport mechanisms in cellulosic materials: Vapor vs. bound water, PNAS Nexus, vol. 3, pgad450 (2024)

Densification Of Mesoporous Silicas By Radiation Effects

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Keywords: Mesoporous silica, Radiation damage, Compaction

In recent years, mesoporous silicas (SBA15, MCM41) discovered in the 1990s [1] have been the subject of numerous studies for various applications in the field of catalysis, CO_2 encapsulation, or treatment of radioactive effluents. A new strategy for this treatment is based on the use of a mesoporous silica functionalized by an organic ligand selective of the RadioNuclides (RN). This hybrid material would allow at the same time the separation of the RN and their encapsulation after collapsing the porosity. Several ways are being considered to close the mesoporosity: chemical reactions, thermomechanical treatments, and irradiation effects. The collapse of silica mesoporosity by external irradiation has been demonstrated [2]. More recently, the possibility of closing the porosity of a mesoporous silica through self-irradiation damage produced by the presence of the short-lived actinide ^{238}Pu has been studied in our laboratory. The results of this work will be presented in the talk.
Hybrid silicas doped with about 10 wt% of ^{239}Pu and ^{238}Pu were elaborated. Small-angle X-ray scattering (SAXS), which is accessible on the SOLEIL synchrotron's MARS beamline, was employed for characterization of these Pu-doped samples. After 27 months of ageing, a decrease in the interplanar (100) distance was observed, indicating a densification of around 10% of the pore volume (Figure 1). The elementary mechanisms responsible for the densification process will be discussed in terms of sintering assisted by irradiation damage, viscous flow...

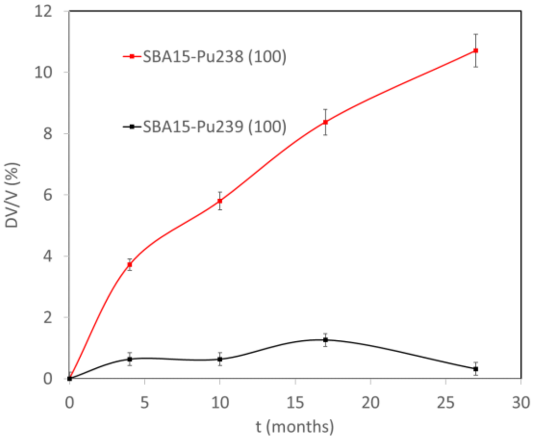

Figure 1: Comparison of the evolution of the volume of the hexagonal cell of ^{238}Pu-SBA15 and ^{239}Pu-SBA15 samples, versus ageing duration. The volume is calculated on the basis of the interplanar (100) distance. ^{239}Pu-SBA15 is used as a reference sample.

References

[1] Beck, J. S., J. C. Vartuli, W. J. Roth, M. E. Leonowicz, C. T. Kresge, K. D. Schmitt, C. T. W. Chu, D. H. Olson, E. W. Sheppard, S. B. Mccullen, J. B. Higgins and J. L. Schlenker, A New Family of Mesoporous Molecular-Sieves Prepared with Liquid-Crystal Templates, American Chemical Society, 114, 1992, 10834-10843 (1992).
[2] Y. Lou, S. Dourdain, C. Rey, Y. Serruys, D. Siméone, N. Mollard, X. Deschanels, Micropor. Mesopor. Mater., 251, 146 (2017).

Porous Media Modeling of Macromolecule Diffusivity in the Intracellular Volume

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Keywords: cell biology; macromolecule diffusion; intracellular medium; upscaling; diffusion measurement; hydrodynamic drag

Transport phenomena in biological systems are essential for maintaining life sustaining functions. Notably, biological materials, including tissues and cells can be viewed as porous media. Here we will focus on the passive transport of macromolecules in the intracellular space involved in many cellular functions, including cell migration, blebbing and apoptosis. While it is well established that intracellular crowding significantly impacts macromolecule mobility, the physical mechanisms by which cytoplasmic structures influence diffusion within the cell remain unclear.

We propose a multiscale diffusion model of the intracellular space based on the volume averaging method. The cytoplasm is treated as a hierarchical porous medium with nanometric and micrometric obstacles. Numerical solution of the model allows us to predict the effective cytoplasmic diffusion coefficient for various obstacle volume fraction. Model predictions are confronted to experimental measurements of the effective diffusion coefficient in live cells and highlight the importance of two key diffusion reduction mechanisms: tortuosity and hydrodynamic drag. Importantly, we find that the effective cytosolic diffusivity is not dependent on specific cellular region but rather on intracellular obstacle volume fraction. Additional model predictions of intracellular diffusivity as a function of the macromolecule size give excellent agreement with literature data.

Altogether, this work demonstrates the potential of porous media modeling approaches to better understand transport phenomena in heterogeneous biological systems all the way to the intracellular scale.

Smooth Particle Hydrodynamics (SPH) code for fracture and hydrofracture propagation

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Keywords : Computational fluid and solid mechanics, fracture mechanics, Soil/structure interaction

In this work, we present a set of simple test cases that illustrate the ability of the Smoothed Particle Hydrodynamics (SPH) method to capture damage initiation and propagation in elastic solids, both in isolation and when coupled to fluid flow. In contrast to alternative approaches, such as phase-field methods solved with finite elements, SPH preserves the local formulation of the damage model, while non-local regularisation naturally arises from the weighted interpolations inherent to the method. Within a unified SPH framework, we discretised the governing equations for fluid flow and infinitesimal-strain solid mechanics and implemented a thermodynamically consistent damage model with unilateral effects [1]. The implementation was first validated on a dynamically loaded, pre-cracked domain, where simulations reproduced crack branching and multi-branching, Fig. 1. The number of secondary cracks was found to depend on the characteristic smoothing length h. We further examined a penny-shaped crack in a purely elastic medium pressurised by fluid. The crack-opening profile obtained with SPH showed excellent agreement with the analytical quasi-static solution. Finally, a simplified hydrofracking test demonstrated that the critical fluid pressure required for damage propagation predicted by SPH lies within 10% of the classical Griffith criterion [2]. These results demonstrate that SPH provides a robust and versatile framework for simulating fracture processes and fluid–solid interactions. In particular, the method holds promise for studying complex scenarios, such as fluid drainage within the realistic pore geometries of natural rocks.

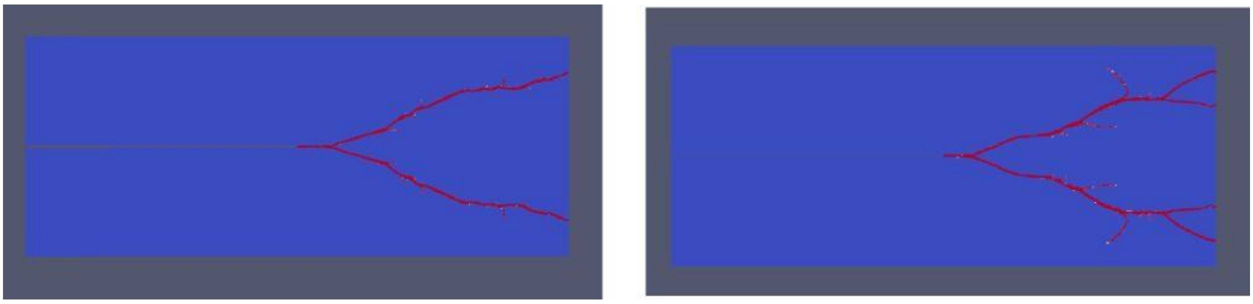

Figure 1: SPH damage patterns with applied stress of $2.5MPa and h=0.25mm for two different initial crack geometries: 2h width with a triangular tip (left) or rectangular with 1h width (right)

References

[1] Deptulski, R. C. (2021). Modélisation des écoulements diphasiques à l'échelle des pores dans des milieux déformables à l'aide de méthodes particulaires (SPH). PhD thesis, Sorbonne University, Paris.

[2] Amrofel, N. (2024), Caractérisation numérique des phénomènes de couplage multiphysique sur la migration de gaz dans une roche argileuse saturée aux échelles mésoscopiques,PhD thesis,Université de Lorraine, Nancy

Bioclogging and its impact on biodegradation in NAPL-contaminated sites

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Keywords: Bioremediation, bioclogging, reactive transport, two-phase flow, numerical modeling

Abstract

Bioremediation of soil contaminated by non-aqueous phase liquids (NAPLs) remains a complex process due to the dynamic interactions between physical, chemical and biological processes. One of the main challenges is pore-clogging, or bioclogging, where biofilm formation within the soil reduces permeability, which in turn affects fluid injectivity and nutrient transport. While microbial activity is essential for contaminant degradation, excessive biofilm formation limits this process. This study presents a mathematical and numerical model that couples two-phase flow, bioreactive transport, and biofilm dynamics, including biomass growth, decay, attachment, and detachment. The model is used to assess how variations in flow rate and nutrient availability influence biofilm development and the associated loss of injectivity. Our findings indicate that optimizing these parameters helps balance the microbial dynamic and minimize bioclogging, thus ensuring continuous biodegradation.

References

[1] Ebigbo A, Helmig R, Cunningham AB, Class H, Gerlach R. Modelling biofilm growth in the presence of carbon dioxide and water flow in the subsurface. Advances in Water Resources. 2010 Jul 1;33(7):762-81.

[2] Thullner M, Schroth MH, Zeyer J, Kinzelbach W. Modeling of a microbial growth experiment with bioclogging in a two-dimensional saturated porous media flow field. Journal of contaminant hydrology. 2004 May 1;70(1-2):37-62.

[3] Soulaine C, Pavuluri S, Claret F, Tournassat C. porousMedia4Foam: Multi-scale open-source platform for hydro-geochemical simulations with OpenFOAM®. Environmental Modelling and Software. 2021 Nov 1;145:105199.

Development of a New Well-Balanced Numerical Scheme for Compressible Porous Media Flows

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Keywords: compressible flow, porous media, well-balanced schemes, low Mach number, AMR, Darcy Forchheimer model

The modeling and simulation of compressible flows in porous media is a dynamic and interdisciplinary field of study. Its applications range from natural phenomena such as groundwater flow, geothermal energy extraction and gas migration to industrial processes like filtration systems, enhanced oil recovery and fuel cell technology. The modeling of such flows is particularly challenging due to the interplay between complex physical phenomena. Indeed, it is critical to account for spatial and temporal variations in porosity and permeability. Moreover in many application, it is important to guarantee that physical properties are preserved like mass conservation, or stability properties related to energy or positivity of the mass.

To address these challenges, we developed a new well-balanced numerical method [1] for compressible flows in porous media, using the superficial velocity as the primary variable instead of the microscopic velocity. This method, relies on a second-order (with respect to space) cell-centered finite-volume discretization implemented in the CanoP code [2]-[3]. Our discretization strategy ensures the conservation of mass, momentum, and energy, while maintaining consistency between the pressure gradient and other source terms. This is critical for achieving accurate simulations in regions with varying porosity and permeability. Additionally, the numerical method employs Adaptive Mesh Re-finement (AMR) [4] strategy to efficiently handle sharp gradients and variations of the porosity.

Our method is tested against test cases of the literature [5], such as the flow through a porous plug, the Beavers and Joseph problem, and flow over a porous square cylinder (see Figure 1). These tests demonstrated the robustness and accuracy of our approach, improving the precision around sharp interfaces by two order of magnitudes compared to previous works. In future work, we plan to extend the application of this scheme to industrial processes, including hydrogen production through water electrolysis, highlighting the potential of the method to advance energy-related technologies.

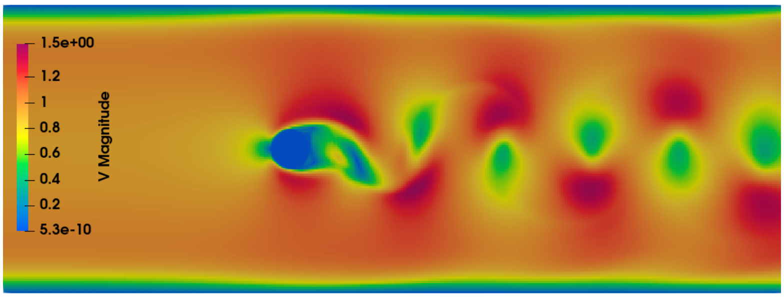

Figure 1: Flow over a porous cylinder: Velocity contours of the porous cylinder with observation of the Von Karman vortex.

References

[1] Chalons et al., A large time-step and well-balanced Lagrange-projection type scheme for the shallow water equations, Communications in Mathematical Sciences, 3, 65-788 (2017)

[2] Fang Chen, Modélisation d'un jet de gaz dans le collecteur sodium des échangeurs á plaques compacts sodium gaz des réacteurs nucléaires de la filiére RNR-Na, Doctoral thesis, (2019)

[3] `https://canop.readthedocs.io/en/latest/`

[4] Isaac et al, Recursive algorithms for distributed forests of octrees., SIAM Journal on Scientific Computing 37, C497-C53 (2015)

[5] Li et al, Implementation of compressible porous fluid coupling method in an aerodynamics and aeroacoustics code part I: Laminar flow, Applied Mathematics and Computation, 364, 124682 (2020)

Enhancements in Large-Scale Subsurface Flow Modelling

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***Keywords**: Groundwater, Saturation, Richards equations, Dupuit-Forchheimer,* Infiltration modelling, Aquifer dynamic

The general context of this work is the development of a numerical strategy to improve the modelling of the hydrological response of a catchment on a multi-decadal scale. At the spatial and temporal scales considered, surface runoff cannot be accurately described by surface processes alone, due to its active coupling with subsurface flow (the groundwater system) [1]. To successfully integrate these couplings, it is necessary to correctly describe the variables that will control the exchanges. That is the reason why it is crucial to simulate not only the groundwater system, but also the dynamics of the unsaturated zone.

However, modelling groundwater flow involves complex interactions between infiltration processes and aquifer dynamics. Richards' equation accurately models both unsaturated and saturated flow, including infiltration processes, but is computationally expensive when applied over large three-dimensional domains, particularly due to the strong non-linearity of the equations [2]. Therefore, the objective of this work is to enhance the computational efficiency of subsurface water flow modelling at large temporal and spatial scales.

The core idea of this research is, through a set of reasonable assumptions, to divide the two dominant physical processes: the infiltration and the aquifer dynamic, where the first one is described by a one-dimensional congested Richards equation in the vertical direction (z-axis) [3], and the second one by the Dupuit-Forchheimer type equation in the horizontal plane ((x, y)-axes). This decomposition assumes that flow in the unsaturated zone is predominantly vertical, while flow within the saturated aquifer is considered primarily horizontal, which is justified by a low shallowness number. These two models are then coupled through a source term that ensures mass conservation. It has to be kept in mind that this approach may lead to some limitations in accurately representing few complex hydrogeological configurations, but this approach approximates well the three-dimensional groundwater flow using a multi-directional framework, which is computationally very efficient.

References

[1] Camporese & al., Surface-subsurface flow modeling with path-based runoff routing, boundary condition-based coupling, and assimilation of multisource observation data, *Water Resources Research*, 46.2, p.1-22 (2010).
[2] Cockett & al., *efficient 3D inversions using the Richards equation, Computer & Geosciences*, 116, p.91-102 (2018).
[3] Brenner and Cancès, i*mproving Newton's Method Performance by Parametrization: The Case of the Richards Equation*, SIAM Journal on Numerical Analysis, 55.4, p.1760-1785, (2017).

Studying Diffusiophoresis-Driven Colloid Transport in Porous Media Using Microfluidics

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Keywords: diffusiophoresis, porous media, colloid, microfluidics

The remediation of contaminated soils and groundwater is a major challenge. A promising approach exploits colloids movement under the effect of solute concentration gradient generated in situ **[1]**. This phenomenon, called diffusiophoresis, offers considerable potential to direct colloids toward areas of the porous microstructure that would otherwise be inaccessible (e.g. dead-end pores). However, diffusiophoretic transport in geological porous media has received very little attention to date, particularly in standard transport models, where this phenomenon is often overlooked. In most cases, studies are carried out on simple geometries, while the few investigations on complex geometries are mainly based on theoretical modeling **[2]**.

The objective of this study is to better understand the diffusiophoretic transport of colloids in complex porous media, using microfluidic devices designed to replicate the geometries of natural environments. These devices allow direct observation of colloid displacement and the analysis of transport mechanisms at the pore scale. Experiments are conducted with and without concentration gradients to compare migration dynamics. The impact of local conditions on colloid behavior—such as the structure of the porous medium or the presence of dissolved chemical compounds—is also assessed. The tracking of colloids is ensured through high-resolution imaging techniques combined with advanced image processing algorithms to quantify the dynamics of movement and migration. The expected results should reveal significant differences in the behavior of colloids transport in the presence of concentration gradients in porous media **[2]**. This effect will be quantified both at the pore scale and by examining particle transport on a global scale. These results contribute to the design of new methods for groundwater remediation by enabling more precise control over colloid transport toward specific contaminated areas.

References

[1] B. V. Derjaguin, G. Sidorenkov, E. Zubashchenko, et E. Kiseleva, « Kinetic Phenomena in the boundary layers of liquids 1. the capillary osmosis », *Prog. Surf. Sci.*, vol. 43, n° 1, p. 138‑ 152, 1947, doi: 10.1016/0079-6816(93)90023-O.

[2] M. Jotkar, P. de Anna, M. Dentz, et L. Cueto-Felgueroso, « The impact of diffusiophoresis on hydrodynamic dispersion and filtration in porous media », *J. Fluid Mech.*, vol. 991, p. A8, juill. 2024, doi: 10.1017/jfm.2024.546.

Conduction–Radiation Coupling : Characterization Of The Effective Thermal Properties of Geopolymers

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Keywords: geopolymer foam, thermal conductivity, conduction-radiation coupling, Monte Carlo method

Global population growth leads to an increase in energy demand, encouraging the use of renewable energy sources such as biomass, which remains essential for cooking. However, the scarcity and inefficient use of biomass necessitate the optimization of thermal efficiency in stoves and cookers various studies [1–3] have aimed to identify the most efficient stove models among the most commonly used, based on the Water Boiling Test (WBT) protocol. However, stove optimization can be achieved not alone through performance comparison, but by improving their components.

This work focuses on obtaining the thermal properties of a geopolymer: a foam made from Bangeli clay [4]. The first part is devoted to the experimental characterisation of the geometric and thermal properties of the geopolymers previously prepared (Sample $^{20.5}C^{2.75}$: apparent porosity 65%, apparent heat capacity 1497 ± 10% $J.kg^{-1}.K^{-1}$, apparent thermal conductivity 0.18 ± 10% $W.m^{-1}.K^{-1}$, real density 2429 ± 1% $kg.m^{-3}$). These data are compared with those obtained from 3D reconstructions of samples, based on tomographic images and those calculated on this geometry. Geometric properties such as porosity, specific surface area, pore size distribution and tortuosity were determined using the 3D reconstruction with iMorph software.The analysis of the coupled conductive-radiative heat transfer is performed using the Monte Carlo Method based on path space formulation via the open source Stardis [5] because geometric complexity does not impact the computational time and it works directely on the 3D surface mesh [6-7].

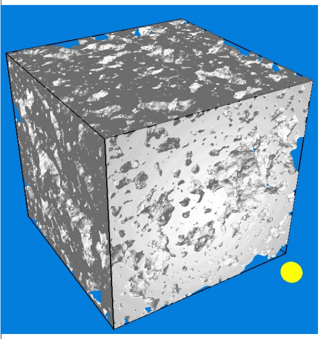

Figure 1: Bangeli Clay Reconstructed 3D image

This study examines the effective thermal conductivity in pure conduction and in conduction-radiation coupling, while assessing the influence of thermophysical properties (conductivity, heat capacity) on the latter (in stationary mode). A comparison between numerical results and experimental measurements is presented.

References :

[1] Segbefia E. et al., «Comparaison de la performance de deux types de foyers améliorés traditionnels : foyer à argile du togo et foyer malgache». Journal de la Recherche Scientifique de l'Université de Lomé, (2018)

[2] Anjorin M. et al., «Étude économique des foyers domestiques par la technique d'ébullition de l'eau : cas du Bénin» Revue Internationale des Sciences et Technologie, (2014).

[3] Abasiryu et al. «Performance evaluation of some locally fabricated cookstoves in Mubi, AdamawaState, Nigeria», Nigerian Journal of Technology 48-53 (2016).

[4] Hounsi A. «Géomatériaux pour l'éco-construction : Synthèse et caractérisation de matériaux géopolymères à base d'argiles» Thèse, 2013.

[5] Stardis https://www.meso-star.com/projects/stardis/stardis.html

[6] Bati M. et al., «Coupling Conduction, Convection and Radiative Transfer in a Single Path-Space: Application to Infrared Rendering», ACM Trans. Graph., vol. 42, p. 79:1-79:20, (2023).

[7] Sans M. et al., "Solving transient coupled conductive and radiative transfers in porous media with a Monte Carlo Method," *Int. J. Therm. Sci.*, 179 (2022).

Simulation Of Reactive Transport Dynamics In Cerebral Microcirculation

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Keywords: Blood microcirculation, Multi-scale modelling, Anomalous transport

Cerebral function is highly dependent on a continuous blood supply of oxygen and nutrient. Depending on its duration and intensity, any disruption of blood supply can lead to progressive neurodegeneration and cognitive decline. For instance, Alzheimer's disease (AD) patients are subject to a chronic decrease of cerebral blood flow (CBF) which is believed to induce tissue hypoxia and further neurodegeneration. The physical mechanisms shaping the distribution of hypoxic regions are still poorly understood.

In this context, a theoretical framework based on the statistical distribution of quantities derived from intravascular blood flow and transport simulations has been developed [1]. Its main advantage is that it quantitatively relates transport dynamics to the network architecture and flow distributions. However, oxygen transport and consumption in the tissue is currently overlooked. Here, in order to subsequently enrich this theoretical framework, we develop a complete coupled model for extravascular and intravascular transport by generalizing to 3D the operator splitting approach introduced in 2D in [2] and by coupling it with an averaged 1D intravascular model with effective coefficients modeling dispersive effects and exchanges with surrounding tissues [3]. In the long term, we expect that the accurate modelling of tissue/vessel couplings should significantly affect the relationship between network topology and the distribution of hypoxic regions.

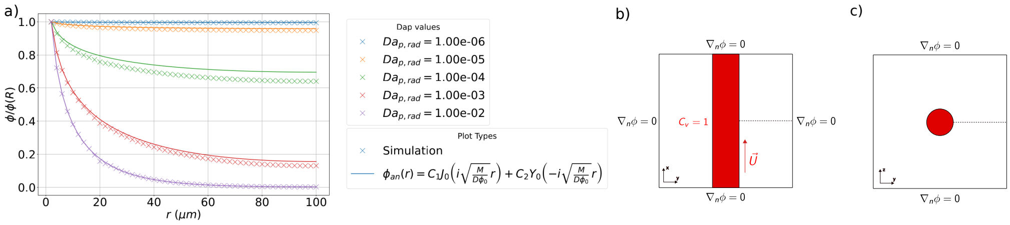

Figure 1: **a)** : Simulated extravascular concentration profiles for a single vessel (×) compared with the analytical solution (continuous line). Tissue with linear metabolism. Different metabolism regimes are shown. ($Da_{p,rad} = \frac{MR^2}{\phi_0 D_p}$)
b) & c) : Schematic representation of the boundary problem whose solutions are shown in **a)**, the dotted line shows the radius for which the solutions have been plotted.

We first validate this numerical framework by comparison with analytical solutions in relevant asymptotic cases. We then use it to identify the physical regime for which the first-order intravascular approach remains valid.

References

[1] Florian Goirand, Network-driven anomalous transport is a fundamental component of brain microvascular dysfunction, Nature Communications, Volume 12 (2021)
[2] David Pastor-Alonso, Modeling oxygen transport in the brain: An efficient coarse-grid approach to capture perivascular gradients in the parenchyma, PLOS Computational Biology, Volume 20 (2024)
[3] Maxime Berg, Modelling solute transport in the brain microcirculation: is it really well mixed inside the blood vessels?, JFM, Volume 884 (2020)

Water Retention Curve of PEM Fuel Cell Catalyst Layer From Numerical Simulations On 3D Digital Images

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Keywords: PEMFC, FIB-SEM, Mixed wettability, Water retention curve

This work aims at determining a key-property of a PEMFC cathode catalyst layer (CCL): its water retention curve (WRC). The latter is highly dependent on the wettability properties of the CCL, which in turn are dependent on the ionomer distribution in the CCL. Starting from a CCL voxelized image obtained by FIB-SEM, a first step is to reconstruct the ionomer distribution in the image following[1], example Fig 1. Then after partition of the pore space in individual pores using a watershed algorithm [2], an effective contact angle is determined for each pore [3]. This confirms that the CCL is a nanoporous medium of mixed wettability with a mean contact angle close to 90°. Then, the WRC is computed using a full morphology approach [4] and a pore network model [2]. Results from both approaches are compared and discussed from comparisons with data from literature.

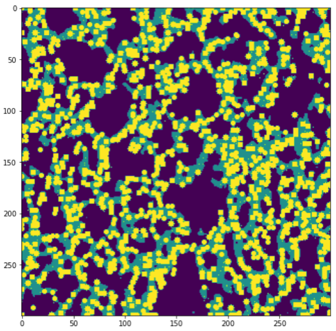

Figure 1: Slice of CCL after reconstruction with ionomer in turquoise blue, carbon grains in yellow and pores in dark purple.

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References

[1] M. Ahmed-Maloum al. Characterizing PEM fuel cell catalyst layer properties from high resolution three-dimensional digital images, part I: A numerical procedure for the ionomer distribution reconstruction. International Journal of Hydrogen Energy 80, 39-56 (2024)

[2] J. Gostick et al. PoreSpy: A Python Toolkit for Quantitative Analysis of Porous Media Images. Journal of Open Source Software, 4(37), 1296 (2019)

[3] M. Ahmed-Maloum, M. Quintard, M. Prat. Characterizing PEM fuel cell catalyst layer properties from high resolution three-dimensional digital images, part III: Contact angle distribution. International Journal of Hydrogen Energy 80, 173–187 (2024)

[4] M. Secanell et al. OpenFCST: An open-source mathematical modeling software for polymer electrolyte fuel cells, ECS Transactions, 64(3), 655 (2014).

Attenuation Measurements In Thermally Cracked Fontainebleau Sandstone: A New Dataset

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Keywords: Laboratory measurements, Thermal properties, Elastic properties

Fluid-saturated rocks can strongly attenuate seismic waves. The waves induce pore pressure gradients, and as a result dissipative fluid flow occurs. At the pore scale, this process is known as squirt flow [1], and the associated energy dissipation and velocity dispersion can be observed in the laboratory over a broad frequency range. Knowledge of pore and fracture characteristics and their interconnectivity is of enormous significance to the development and production of geothermal resources as well as for the geological sequestration of CO2.

Three cylindrical samples of 80 mm in length and 40 mm in diameter were cored from the same block of Fontainebleau sandstone: an intact one and two heat-treated samples. The heat treatments were done at 500°C and 625°C, according to the α-β transition temperature of quartz, and resulted in an increase of porosity on both samples [2]. We measured the frequency-dependent elastic moduli and attenuation using the forced oscillation method in a hydraulic triaxial cell installed at the Laboratoire de Géologie of École Normale Supérieure in Paris. We obtained the Young's modulus *E* from the ratio of the stress to that of the resulting axial strain on the sample, and its related dissipation Q_E^{-1} from the phase shift between the applied stress and the resulting strain on the sample. The measurements were made over the frequency range of 0.2 Hz to 200 Hz at Terzaghi's effective pressures from 2.5 MPa to 25 MPa. Pore pressure was maintained at 5 MPa throughout the experiment.

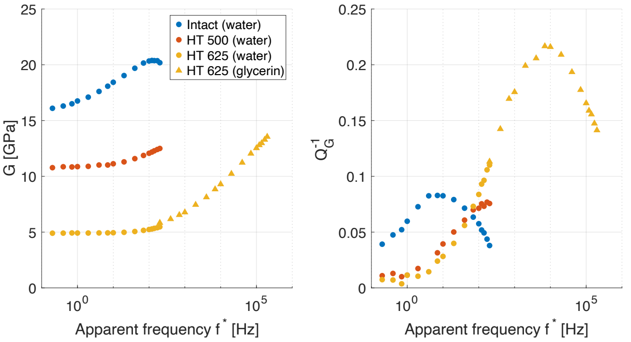

Figure 1: Young's modulus and dissipation measurements at 5 MPa effective pressure on the intact and heat-treated samples.

Our study highlights the frequency-dependent behaviour of attenuation and dispersion measured in fluid-saturated Fontainebleau sandstone, driven by the squirt flow mechanism under undrained conditions. Heat treatment resulted in reduced Young's modulus and increased porosity, attributed to the widening and creation of cracks, which shifted the characteristic frequency of attenuation and dispersion to higher frequencies (Figure 1).

References

[1] Mavko, G., and A. Nur, Melt Squirt in the Asthenosphere., *Journal of Geophysical Research*, 80, 1444–14 (1975).
[2] Darot, M., Y. Gueguen and M.-L. Baratin, Permeability of thermally cracked granite., *Geophysical Research Letters*, 19, 869-872 (1992).

Micro-mechanical Study of Hydro-mechanical Coupling at the Interfaces of Raw Earth Masonry

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Keywords: Hydro-mechanical behavior, raw earth, multi-modal imaging

The use of bio or geo-sourced materials is a sustainable solution to reduce the carbon footprint in the building sector. Among these, raw earth materials stand out thanks to its reversibility, local availability, and remarkable hygrothermal properties. Nevertheless, this material sometimes exhibits unpredictable mechanical responses due to its high sensitivity to water [1], which hinders a more widespread adoption. Raw earth is a composite material whose clay and silt particles, once hydrated, act as a binder for the granular skeleton. The cohesion of this porous medium and its mechanical properties are therefore strongly correlated with its hydric state [2]. During the construction of masonry structures, earth bricks are placed in contact with wet earth mortar, leading to water exchange through capillary flow (imbibition process) and evaporation (drying process) at the brick/mortar interfaces. This results in swelling and shrinkage of the material, which can induce significant local damage (micro-cracking) and severely affect cohesion. The extent of these micro-mechanisms is expected to be controlled by the microstructure and, in particular, by the properties of the pore network. In this work, we characterize the hydromechanical coupling that leads to the cohesion between earth bricks and mortar to explain the counterintuitive observation that walls built with denser bricks, featuring thinner pores and higher capillary forces, may exhibit worse strength than looser bricks with larger pores and lower capillary forces. The response of raw earth structures, including masonry, has primarily been studied at macroscopic and phenomenological levels. To our knowledge, no full-field micro-mechanical study of hydromechanical coupling at interfaces exists, despite the need to understand and quantify these processes at the local scale due to the material's strong intrinsic and induced heterogeneity. In our study, we track the evolution of raw earth microstructures (samples of dimensions $\varnothing \times h = 20 \times 40$ mm) during imbibition and drying tests using 3D operando measurements in a laboratory micro-tomograph as well as the multi-modal (neutron+X-ray) imaging platform NeXT at the institut Laue-Langevin [3]. The combined use of neutron and X-ray tomography allows us to characterize the hydro-mechanical behavior of brick-mortar interface during these processes by locally relating deformation and micro-cracking (visible through X-rays) to the saturation rate (visible with Neutrons). We are also studying the impact of the microstructure on this hydro-mechanical coupling by testing raw earth with different porosity levels, as well as different grain size distributions and mineralogical compositions.

References

[1] Hall M, Djerbib Y Moisture ingress in rammed earth: part 1—the effect of soil particle-size distribution on the rate of capillary suction. Constr Build Mater 18:269–280. (2004)

[2] Chauhan, P., El Hajjar, A., Prime, N., & Plé, O. Unsaturated behavior of rammed earth: Experimentation towards numerical modelling. *Construction and Building Materials*, *227*, 116646 (2019).

[3] Tengattini, A., Lenoir, N., Andò, E., Giroud, B., Atkins, D., Beaucour, J., & Viggiani, G. NeXT-Grenoble, the Neutron and X-ray tomograph in Grenoble. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, *968*, 163939 (2020).

Refined porous ceramic manufacturing using active learning

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***Keywords**:* Powder metallurgy, Porous ceramic, Active learning, Classification, Permeability

Understanding fluid transfer in porous media is necessary to model certain composite material manufacturing processes [1]. Unfortunately, current models do not always correctly predict flow behavior in cases where the porous media is unsaturated, particularly infusion times. Compared to deformable fibrous media, porous ceramic model samples allow limiting and controlling the geometric variability of the porous network. Aiding to isolate the parameters influencing resin impregnation regimes in the material. This study has applications in the medical field (ceramics/polymers). It could also be extended to other types of composites and therefore other fields such as transportation or energy (carbon/epoxy fibers, flax/thermoplastic fibers, etc.).

The medium-term objective is to develop models to better understand fluid transfer in unsaturated porous media [2] and predict filling kinetics based on measurable material parameters. To this end, ongoing work aims to build an experimental database. We developped an active learning algorithm to find the limit process parameters for the manufacturing of porous ceramics, with a limited number of trial-error iterations. The algorithm, which rely on Gaussian Process Regression (GPR), allows to find the best parameters to investigate based on already checked parameters. This is particularly helpful for process with numerous parameters for which a standard experimental plan would take a large amount of time for sample test. We will present the prediction ability of the active learning algorithm for a test case with 2 parameters varying (porogen volume and sizes).

Following this, the permeability of the porous ceramics depending on the process parameters and poral space geometry will be presented and discussed. Instrumented infusion tests are performed to measure the flow rate and pressure during fluid injection. Besides, the samples are characterized by scanning electron microscopy, mercury porosimetry, and X-ray microtomography to understand their internal structure (pore distribution) [3]. This work will help determine the most representative morphological parameters of the porous medium in order to model its fluid-filling kinetics. It will pave the way for a convergence between experimentation and numerical modeling for a better understanding and control of the infusion process.

References

[1] Reaction-bonded B4C/SiC composites synthesized by microwave heating - Dutto - 2019 - International Journal of Applied Ceramic Technology - Wiley Online Library, (n.d.). https://ceramics.onlinelibrary.wiley.com/doi/abs/10.1111/ijac.13211 (accessed April 11, 2025).

[2] L. Xie, Q. You, E. Wang, T. Li, Y. Song, Quantitative characterization of pore size and structural features in ultra-low permeability reservoirs based on X-ray computed tomography, J. Pet. Sci. Eng. 208 (2022) 109733. https://doi.org/10.1016/j.petrol.2021.109733.

[3] S. Nickerson, Y. Shu, D. Zhong, C. Könke, A. Tandia, Permeability of porous ceramics by X-ray CT image analysis, Acta Mater. 172 (2019) 121–130. https://doi.org/10.1016/j.actamat.2019.04.053.

Crystallization Of Sodium Chloride In Microfluidic Pore Systems

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Keywords: Microfluidics, Porous Media, Salt Crystallization, SEM

Salt crystallization in porous media induced by drying is a crucial subject, in connection with many issues such as soil salinization, CO2 injection in saline aquifers [1], material durability or cultural heritage preservation. Previous studies have shown the complexity of the coupling between drying kinetics, wettability of the medium, pore size and salt structure [2]. These structures - such as crusty or patchy efflorescences, subflorescences or compact crystals - can cause damages in the media and modify drying rates, yet the understanding of these phenomena remains insufficient to be predictable.

This work aims at observing sodium chloride subflorescence growth during evaporation in porous media, focusing on the shape and properties of the resulting salt structures (porosity, permeability) depending on pore size and wettability. We develop two-dimensional microfluidic chips mimicking simple porous geometries, allowing optical microscopy observation of crystallization kinetics. The study explores the impact of geometrical confinement and wettability on salt crystallization. Different hydrophilic/hydrophobic patterns are created to stabilize the evaporative front in the porous media and force subflorescence formation. Our microfluidic devices, designed to be reopened after drying, allow further analysis of the remaining crystals through Scanning Electron Microscopy (SEM).

Two types of crystals are observed: monocrystals forming in solution and aggregates developing in dry areas from the liquid front. Moreover, the hydrophilic nature of the crystals drives solution within the aggregates, advancing the wet front into the hydrophobic regions. In perspective, other substrates (PDMS, halite) will be tested to assess surrounding material impact on salt crystals.

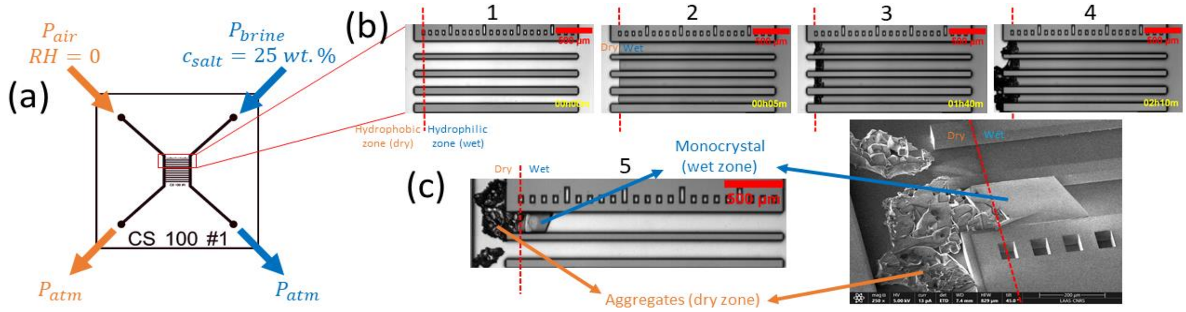

Figure 1: Crystallization process. (a) Schematic representation of saltwater (blue) and dry air (orange) flows within the chip. (b) Zoom on channels (1), chip filling (2), crystals growth during evaporation (3,4). (c) Dried crystals after an experiment (5, t+48h), SEM image.

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References

[1] Kim et al., Aquifer-on-a-Chip: understanding pore-scale salt precipitation dynamics during CO2 sequestration, *Lab on a chip*, 13, 2508-2518 (2013).

[2] Derluyn and Prat, *Salt crystallization in Porous Media*. ISTE-Wiley (2024).

Moisture Behavior in Textiles: A Dynamic NMR Study

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Keywords: NMR relaxometry, textiles, drying, porosity

In textiles, moisture can exist in two main forms: so-called free water, located in the pores, and bound water, which is absorbed within the structure of natural fibers [1], [2]. Although bound water can account for up to 30% of a textile's dry mass, it remains difficult to detect, as the water molecules are dispersed within the amorphous regions of cellulose and therefore escape conventional microscopy techniques. This absorption phenomenon is closely related to the nature of the fibers, whether plant-based (e.g., cotton), animal-based (e.g., wool), or synthetic (e.g., acrylic). Additionally, the textile's structure—whether woven, knitted, or nonwoven—may also influence how water is stored and transported. While thermal transfers in such materials are well understood, moisture-related processes remain comparatively underexplored.

To gain deeper insight into the mechanisms governing water transport in textiles, we focus on the behavior of textile materials or compacted fibers with varying porosities when brought into contact with liquid water. To monitor the different transport phenomena, we employ dynamic NMR relaxometry [3]. This technique allows for the time-resolved analysis of the probability density function of the transverse relaxation time, by examining parameters such as peak integrals, peak widths, and mean relaxation times. These data enable us to distinguish between free and bound water—whose relaxation times differ significantly—assess potential exchanges between these phases, and characterize their distribution within the material. This dynamic monitoring provides key insights into how water behaves depending on the nature of the textile and its porous microstructure. The data in particular show that during the imbibition phase, part of the water is absorbed into the solid matrix as bound water. This is followed by a drying process during which the different forms of water gradually evaporate. We quantify these different processes with the help of a simple diffusion model.

References

[1] X. Ma *et al*., Vapor-sorption Coupled Diffusion in Cellulose Fiber Pile Revealed by Magnetic Resonance Imaging, Physical Review Applied 17 (2022).
[2] C. Duprat, Moisture in Textiles, Annual Review of Fluid Mechanics 54, 443–467 (2022).
[3] B. Maillet *et al*, Dynamic NMR Relaxometry as a Simple Tool for Measuring Liquid Transfers and Characterizing Surface and Structure Evolution in Porous Media, Langmuir 38, 15009−15025 (2022).

Spatio-temporal Characteristics Of A Proliferating *Saccharomyces Cerevisiae* Clog

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Keywords: bioclogging, proliferation, microfluidics

Bioclogging is a process that result from the separation of biological particles from a fluid by a membrane; it has many environmental and sanitary applications. It results in a reactive porous medium with emerging properties: cells are deformable, can proliferate, consume nutrients and oxygen, and die. These specific features affect the structure and behavior of the porous medium. The coupling between proliferation, clog growth, and nutrient consumption can lead to a nutrient-limited environment, altering the proliferation of the organisms [1]. Bioclogging can thus be used to study the dynamics of reactive porous media under environmental constraints. Our objective is to investigate the spatio-temporal features of cell proliferation within a yeast assembly perfused with nutrients at the microscopic scale.

The model organism is *Saccharomyces cerevisiae*. A quasi-2D microfluidic system was developed, in which yeast cells are retained by a pore and continuously perfused with culture medium [2]. Two distinct growth regimes are observed during clog formation, corresponding to different states of the clog. In the initial phase, clog growth is exponential, associated with uniform proliferation throughout the clog. An experiment is presented in figure 1. After a few hours, the clog length evolves linearly with time. Two distinct regions emerge: one proliferative, the other quiescent – as demonstrated by biological marking. We are also able to quantify local proliferation rates within the clog using local displacements. These results highlight the coupling between bioreactive flow and proliferation: growth reduces the flow rate, which in turn reduces the proliferation rate.

A mathematical model has been developed to support the experimental observations. It relies on three key components: a Monod-type proliferation law dependent on nutrient concentration, an advection-diffusion-reaction nutrient transport equation, and a Darcy description of flow through the clog. These equations are coupled to capture the interplay between cell growth, nutrient depletion, and flow reduction. The model successfully reproduces the transition between the observed growth regimes, as well as the emergence of spatially differentiated zones within the clog.

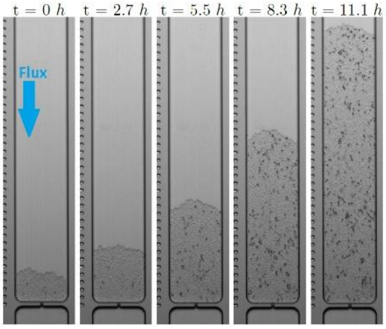

Figure1: Growth of a yeast clog perfused by nutrients

References

[1] Vulin et al., Growing Yeast into Cylindrical Colonies, Biophysical Journal, 106, 2214-2221 (2020)
[2] Desclaux et al., Hydrodynamic resistance of a yeast clog, Physical Review Fluids, 9 (2024)

Multi-scale characterization of the porosity in pretreated lignocellulosic biomass

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Keywords: biomass, porosity, characterization

The transition towards sustainable bio-based processes relies on the efficient conversion of lignocellulosic biomass, a renewable and abundant carbon resource. The biochemical conversion of lignocelluloses into ethanol, through pretreatment, enzymatic hydrolysis and fermentation, has been explored for decades and is nearing maturity. However, hydrolysis remains complex, as its efficiency largely depends on the physico-chemical properties of pretreated biomass. This study develops multi-scale approaches to identify biomass property markers and reactivity, focusing on porous architecture, a key parameter for hydrolysis, as it determines enzyme diffusion before adsorption on cellulose and conversion into glucose. Understanding how porosity influences molecular transport in hydrated biomass is essential for optimizing biomass valorization. We investigate multi-scale porosity in maize stem internodes, considering different genotypes, tissues and pre-treatment conditions [1].
To assess porosity and molecular transport, we use pulsed-field gradient NMR (PFG-NMR) to analyze the diffusion of water and polyethylene glycols (PEGs) probes [2]. Complementary textural analyses, based on adsorption techniques, provide insights into surface properties and pore size distribution. Our results confirm that pretreated samples enhance diffusion, indicating greater cellulosic surface accessibility (fig.1). Diffusion behavior varies with pore structure across tissues, showing clear differences between native and pretreated biomass. It also depends on probe size, revealing mesoporosity's role in enzyme accessibility. By integrating structural imaging techniques, we refine our understanding of cell wall organization [3]. The combined use of diffusion-based and textural characterization provides insights into the structural evolution of lignocellulosic biomass, helping optimize pre-treatment and cultivation strategies for efficient biorefinery processes.

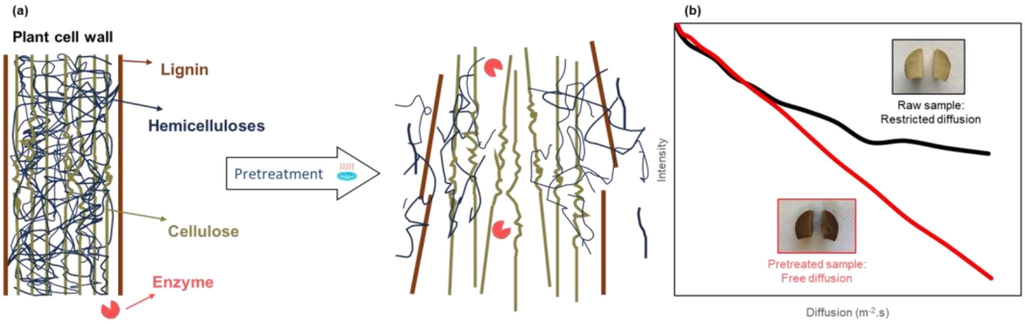

Figure 1: Impact of pretreatment on biomass architecture (a) and PEG diffusion (b).

References

[1] Leroy, A., Falourd, X., Foucat, L. et al., Evaluating polymer interplay after hot water pretreatment to investigate maize stem internode recalcitrance, *Biotechnol Biofuels*, 14, 164 (2021).
[2] Newling, B., Batchelor, S. N., Pulsed Field Gradient NMR Study of the Diffusion of H_2O and Polyethylene Glycol Polymers in the Supramolecular Structure of Wet Cotton, *J. Phys. Chem. B*, 107, 12391–12397 (2003).
[3] Penttilä, P.A., Altgen, M., Carl, N. et al., Moisture-related changes in the nanostructure of woods studied with X-ray and neutron scattering, *Cellulose*, 27, 71–87 (2020).

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Impact of Saturation Level and Water Redistribution on Carbon Mineralization in Unsaturated Porous Media

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Keywords: Unsaturated porous media, Carbon mineralization, Petrophysical properties

Carbon mineralization of mine tailings in the unsaturated zone offers an effective and sustainable solution for CO_2 storage [1], where water content in the porous medium fluctuates due to evaporation [2] and chemical reactions. While carbonation processes have been widely studied, the behavior under very low water content (potentially impacted by capillary conditions) remains largely unexplored. Furthermore, the effects of carbonation on the pore size distribution and therefore on the porosity-permeability relationship is largely overlooked. In this study, we investigated how water saturation affects the carbonation reaction in unsaturated sand-brucite columns. Column experiments were conducted at different saturation levels (30%, 15%, 5%, and 1%), with CO_2 injected from the bottom. CO_2 breakthrough analyses and recorded mass gain revealed that while carbonation is strongly dependent on water content, it remains active even under extremely dry conditions. Additionally, CO_2 injection following prolonged evaporation resulted in a heterogeneous carbonation pattern, driven by water redistribution within the column due to evaporation. Post-mortem scanning electron microscopy (SEM) analysis confirmed the strong influence of saturation level on the extent and nature of precipitated carbonates. The development of secondary nanoscale porosity indicates that the water storage becomes both more efficient and more localized with time, drastically changing the pathway and the mass balance of any gas storage. These findings demonstrate that water saturation affects the carbonation reaction in a non-linear way, and that water distribution plays a critical role in the reaction dynamics. Understanding these coupled effects (water saturation/distribution) is essential for reliable predictions in subsurface applications such as CO_2 storage, geothermal and energy storage systems, and arid soil management.

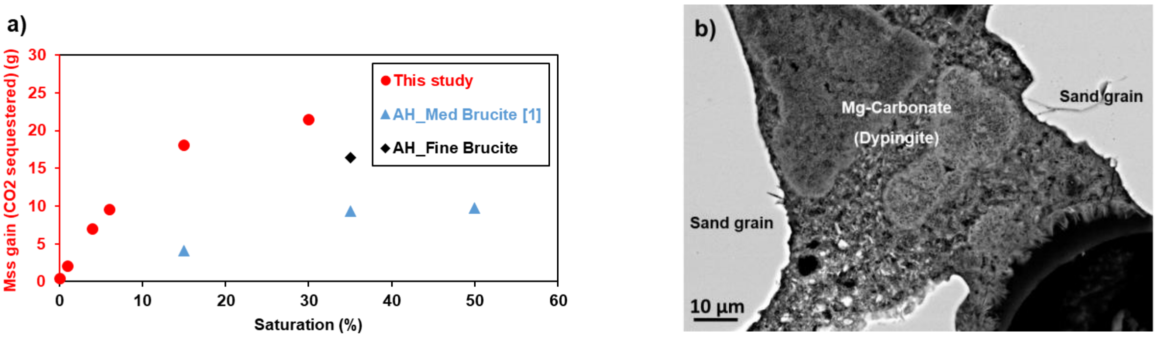

Figure 1: a) Effect of saturation on the extent of carbonation and CO_2 sequestration at column scale. b) Post-mortem SEM image in BSE mode of the sample taken from the column at 30% saturation.

References

[1] A. L. Harrison, G. M. Dipple, I. M. Power, and K. U. Mayer, “The impact of evolving mineral–water–gas interfacial areas on mineral–fluid reaction rates in unsaturated porous media,” Chem Geol, vol. 421, pp. 65–80, Feb. 2016, doi: 10.1016/J.CHEMGEO.2015.12.005.

[2] M. A. B. Zanoni, J. Wang, J. L. Torero, and J. I. Gerhard, “Multiphase modelling of water evaporation and condensation in an air-heated porous medium,” Appl Therm Eng, vol. 212, p. 118516, Jul. 2022, doi: 10.1016/J.APPLTHERMALENG.2022.118516.

Gas transport through porous media induced by a temperature gradient

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Keywords: gas flow, temperature gradient, molecular mean free path, Knudsen number

Under rarefied conditions, *i.e.* at low pressure or when the characteristic flow dimension is small (such as in microchannels or microporous media *etc.*), a temperature gradient along a solid surface bounding the fluid induce gas to flow in the direction of the gradient, namely from the cold side to the hot side. This phenomenon is known as thermal transpiration or thermal creep, first discovered by Reynolds [1], then studied by Maxwell [2], and after by Knudsen [3].

Thermal transpiration occurs when a temperature difference is applied to a gas under rarefied condition and initial pressure equilibrium. Under these conditions, the gas macroscopically moves from the colder region to the hotter one. This phenomenon has recently, garnered renewed interest due to the rapid development of the micro-and nano-technologies [4]. Its effects can be beneficial - such as enabling flow driven solely by a temperature gradient - or detrimental, for instance, when it causes undesired flow within a pressure sensor, potentially distorting measurements.

In our experiments, we aim to measure the gas mass flow rate through a sample consisting of 3600 parallel capillaries (diameter $D = 6\mu$m, length $L = 5$ cm), subjected to a controlled temperature gradient at both ends. This configuration serves as a model of a microporous medium.

The experimental setup consists of a reservoir and a pressure gauge on each side of the sample. A differential pressure gauge is positioned between the two reservoirs to monitor pressure differences. Temperature is controlled using an electric resistor at the hot end and a thermal bath at the cold end. Several thermocouples are installed along the setup to record the temperature profile. The reservoirs are connected by a controllable bypass valve, and the experimental protocol is divided into several phases. Initially, the bypass valve remains open until steady-state conditions are achieved, characterized by equal pressure on both sides. Once equilibrium is established, the bypass valve is closed to begin the experiment. The imposed temperature difference across the sample causes gas molecules to migrate from the cold side to the hot side, generating a pressure difference. This pressure gradient exerts a force opposite to the molecular flow direction. Over time, the increasing pressure difference slows down the molecular transport, eventually leading to a new steady state. The maximum pressure difference reached during this stage is referred to as the thermomolecular pressure difference (TPD). Another key parameter is the characteristic time, which describes the dynamics of the pressure evolution after the bypass is closed.

The mass flow rate, characteristic time, and TPD are measured for various gases and their mixtures. Additionally, expressions are proposed to estimate these parameters as functions of the temperature difference applied across the sample.

References

[1] O. Reynolds, On certain dimensional properties of matter in the gaseous state, Philos. Trans. R. Soc. London 170 (1879) 727–845.

[2] J. C. Maxwell, On stress in rarefied gases arising from inequalities of temperature, Phil. Trans. R. Soc. Lond. 170 (1879) 231–256.

[3] M. Knudsen, Eine revision der gleichgewichtsbedingung der gase. thermische mlekularstömung, Annalen der Physik 31 (1910) 205–229.

[4] M. V. Johansson, H. Yamaguchi, P. Perrier, I. Graur, Some properties of a gas flow submitted to a temperature gradient, International Journal of Heat and Mass transfert 214 (2023) 124372.

Experimental study of heterogeneous reactive transport in unsaturated flows through 3D porous media

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Keywords: heterogeneous, *reactive-transport, air-water and solid-water interfaces, unsaturated flows*

Here, we study the properties of multiphase flow in the vadose zone, which consist of saturated, unsaturated, mobile and immobile regions. This zone is of critical importance because it plays a key role in the transport of water from the surface to the aquifers. It is strongly affected by human activities with the transport of contaminants.

In order to predict the fate of contaminants in natural aquifers and improve remediation solutions, an accurate understanding of the interplay between reactivity and transport at both the micro and macro (Darcy) scale is required.

The macroscale description of reactive transport is generally used [1], but recent studies show that fluid-solid reactivity can be affected by microscale mixing conditions, even in saturated flow conditions [2]. The understanding of these phenomena for heterogeneous reactions in unsaturated media still lacks experimental data that can be further used to support models and simulations [3].

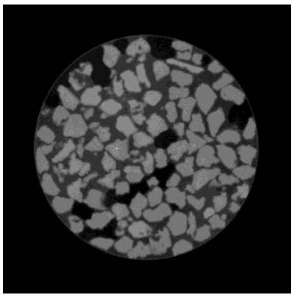

Figure 1: Multiphase porous media picture captured by X-ray microtomography (gas phase in dark, liquid phase in strong grey and solid phase in light grey)

The impact of flow, saturation and structure of the porous media on the transport and the heterogeneous chemistry will be studied along this path. Imaging technologies (XMT, FIL and SPIM) combined with 3D dynamic breakthrough experiments are investigated to open the black box that is porous media (figure 1).

[1] A. E. Scheidegger, « General theory of dispersion in porous media », *J. Geophys. Res.*, vol. 66, nº 10, p. 3273-3278, oct. 1961, doi: 10.1029/JZ066i010p03273.

[2] T. Aquino, T. Le Borgne, et J. Heyman, « Fluid–Solid Reaction in Porous Media as a Chaotic Restart Process », *Phys. Rev. Lett.*, vol. 130, nº 26, p. 264001, juin 2023, doi: 10.1103/PhysRevLett.130.264001.

[3] I. Markale, A. Velásquez-Parra, A. Alcolea, et J. Jimenez-Martinez, « Mixing Controlled Adsorption at the Liquid-Solid Interfaces in Unsaturated Porous Media », *Transp. Porous Media*, vol. 146, nº 1-2, p. 159-175, janv. 2023, doi: 10.1007/s11242-022-01747-x.

Dispersion in Porous Media: A Comprehensive Numerical Comparison of Existing Methods

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Keywords: porous media, dispersion, numerical simulations,

Dispersion in porous media has been of great importance in many engineering fields since decades. In petroleum engineering and environmental applications, various chemicals are injected into reservoirs enhancing oil recovery [1], utilizing the principle of hydrodynamic dispersion. In fluid mixing, depending on the Peclet number (Pe), fluid dispersion could dominate over diffusion thus, accelerating the mass transfer by the local enhancement of concentration gradients [2]. Hence, scientists have for decades tried to describe the complex influence of dispersion on those and other physical processes through experimental and numerical analysis. Unlike simple capillary flows, the dispersion in porous media is also influenced by the complexity of the flow paths. The intensity of the dispersion tends to increase also with the complexity of the porous medium geometry due to the presence of dead-ends, preferential paths, increased fluid spreading and pore connectivity. At the macroscopic level, dispersion can be quantitatively described using an advection dispersion equation associated to Ficks law, with the appropriate transverse and longitudinal dispersion coefficients [3]. In order to calculate the dispersion tensor one could use the volume averaging theory proposed in [4], solving a closure problem whose solution gives the value of the dispersion tensor. The latter is valid only for periodic porous media. Furthermore, numerical tools allow also the use of classical approaches such as the Taylor-Aris dispersion model (derived originally for capillaries) also in porous media [5]. The present work aims to compare the aforementioned methods for obtaining dispersion tensor in porous media. Although the topic of fluid dispersion in porous media has been studied for decades, to the best of our knowledge, there is no comprehensive comparative analysis of the used dispersion models in complex porous geometries.

As a reference case, we consider a geometry with well-characterized structural and flow properties, using the Kelvin cell structure as an example, which has been previously analyzed in detail in [6]. As a representative example of a disordered porous medium, we employ the geometry introduced in [7], where a simple sugar cube was used as a template to create a random pore network made of polydimethylsiloxane (PDMS) polymer, originally used for the purpose of on-chip microfluidic mixing. The main idea of the present work is to compare various approaches for quantifying fluid dispersion in a disordered porous structure, with a particular focus on their assumptions and limitations (e.g., the requirement of fully developed dispersion in the Taylor method). Using fluid mixing as a reference application, different dispersion regimes will be analyzed, and the influence of dispersion intensity on the overall mixing behavior will be examined.

References

[1] N. Pham, et al. Bulk stress distributions in the pore space of sphere-packed beds under Darcy flow conditions. Phys. Rev. E Stat. Nonlinear Soft Matter Phys. 89, 1-13, (2014)

[2] Rousseau, Gauthier et al., Dispersion Versus Diffusion in Mixing Fronts, Water Resources Research, 59, 11, 0043-1397, (2023)

[3] Bear J., Dynamics of fluids in porous media, Elsevier, New York, (1972)

[4] Whitaker S., The method of volume averaging, theory and applications of transport in porous media, Kluwer Academic, Dorderecht, (1999)

[5] J.L. Auriault et al., Taylor dispersion in porous media: Analysis by multiple scale expansions, Advances in Water Resources, 18, 4, 217-226, (1995)

[6] Yann Jobic, et all. Determining permeability tensors of porous media: A novel vector kinetic numerical approach. International Journal of Multiphase Flow , 110, pp.198-217, (2019)

[7] Emil Grigorov, et al., Novel Approach for Passive Mixing in Microfluidics Utilizing Porous PDMS Sponge, Int. Sc. Conf. Comp. Sc., 2, 1-6, (2023).

Influence of Wettability on Water Relative Permeabilities Curves in Unconsolidated Porous Media: From Water-wet to Oil-wet

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Keywords: Fractionally wet, van Genuchten model, water retention curves

Laboratory column experiments were conducted to investigate the influence of wettability on water relative permeability (k_{rw}) as a function of water saturation (S) in unconsolidated porous media. Wettability conditions varying from water-wet to oil-wet, including intermediate states, were systematically explored. Accurate characterisation of wettability effects is essential for modelling multiphase flow in systems relevant to hydrogeology, petroleum engineering, and environmental remediation.

The experimental methodology expanded upon a previously developed approach. Localised water content was measured using a PICO TDR probe, and pressure gradients were obtained via two pressure transducers placed along the sand-filled columns. This configuration allowed direct measurement of pressure gradients, eliminating the need to impose a unit hydraulic gradient and thereby improving the accuracy of permeability measurements under steady-state flow conditions. Fine and coarse sands were used in all experiments, and wettability was systematically modified through surface treatments to produce water-wet, oil-wet, and fractionally-wet configurations. A constant water flux was imposed at the column inlet, and the resulting pressure differences were monitored along the flow path. Absolute water permeability (K_w) was calculated using Darcy's law at various saturation levels. Water relative permeability (k_{rw}) was then obtained by normalising each K_w with respect to the permeability measured at the maximum water saturation achieved after primary drainage and imbibition at the so-called matching point ($k_{rw,\ mp}$). Fractionally-wet conditions were achieved by mixing water-wet and oil-wet grains in controlled proportions. The k_{rw}–S curves are analysed for variations in both shape and magnitude depending on wettability. The analysis focusses on potential differences in hysteresis effects observed during drainage and imbibition.

The initial results for water-wet sands indicated that the experimental k_{rw}–S relationships obtained during drainage were well captured by the Van Genuchten model, with the fitting parameters successfully derived from the corresponding water retention curves. Future work will include numerical simulations at the pore scale using X-ray tomography images of the porous media. These simulations will be conducted in OpenFOAM to further analyse flow dynamics and validate experimental findings.

Data-Driven Prediction of Oil Removal Efficiency in Surfactant-Enhanced Remediation

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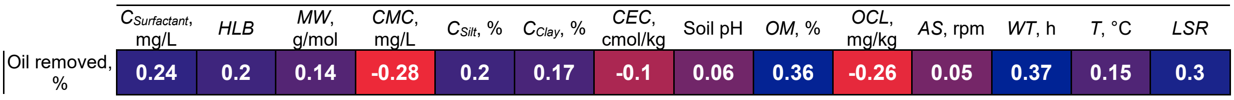
Keywords: Machine learning; Oil removal; Surfactant-enhanced remediation

As an effective means of removing petroleum hydrocarbons from contaminated soils, surfactant-enhanced remediation (SER) increases solubilization and desorption [1]. The nonlinear interactions that govern SER efficiency between soil, contaminants, and surfactants are not fully captured by conventional empirical and mechanistic models. Such complexity may be modeled effectively using machine learning (ML) approaches. This study evaluated three regression algorithms not previously evaluated: light gradient boosting machine (LGBM), extra-trees regression (ETR), and k-nearest neighbors (KNN) on a database of 2,394 experimental records collected from almost 50 SER studies. We reduced the data points to 1,891 by removing 503 outliers (21%), screening for multicollinearity, and scaling inputs. Feature sets with redundancy or negligible predictive value were excluded (e.g., asphaltene fraction, sand content) [2]. Using GridSearchCV, the hyperparameters of models were tuned by dividing the cleaned database into training (80%) and test (20%) sets. A preprocessed correlation matrix demonstrating multicollinearity control is shown in Figure 1. All three algorithms demonstrated strong predictions. LGBM and KNN were outperformed by ETR with an R² = 0.984, RMSE = 2.658, and MAE = 1.257 on the entire set of data.



	$C_{Surfactant}$, mg/L	*HLB*	*MW*, g/mol	*CMC*, mg/L	C_{Silt}, %	C_{Clay}, %	*CEC*, cmol/kg	Soil pH	*OM*, %	*OCL*, mg/kg	*AS*, rpm	*WT*, h	*T*, °C	*LSR*
Oil removed, %	0.24	0.2	0.14	-0.28	0.2	0.17	-0.1	0.06	0.36	-0.26	0.05	0.37	0.15	0.3

Figure 1: Spearman correlation heatmap used to identify collinear features in the dataset.

Figure 2 illustrates that, while the ETR and LGBM predictions are close to a 1:1 line, the KNN predictions display a greater degree of scatter.

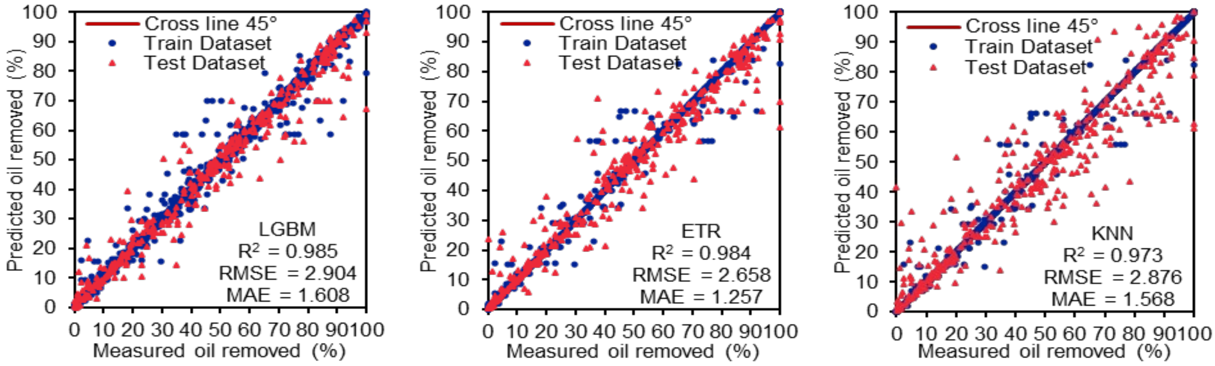


Figure 2: Cross plots of predicted vs. measured oil removal (%) for trained models.

These results highlight the stability of the ensemble methods, particularly the ETR, for predicting SER efficiency. Additionally, data-driven modeling may reduce the need for trial-and-error approaches and encourage cost-effective, sustainable remediation strategies by identifying the optimal surfactant and operational parameters.

References

[1] K. Urum, T. Pekdemir, Evaluation of biosurfactants for crude oil contaminated soil washing. Chemosphere 57(9), 1139–1150 (2004).

[2] E. Hajibolouri, B. Bekbau, S. Omirbekov, M. Ranjbaran, D. Turalina, M. Riazi, New Smart Models for Predicting the Effect of Surfactants on Oil Removal from Soil Contamination Using Experimental Data. SSRN Preprint 5381526 (2025).

Water transfers in starch-fibers composites

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[a]*Navier Laboratory, Gustave Eiffel University*

Keywords: Starch, natural fibers, bio-based materials, hygrothermal behavior, porous media

In the push for biodegradable and environmentally friendly material in the construction field, bio-based materials like natural fibers are stealing the spotlight. They're not only kinder to the planet with lower CO_2 emissions but also act as natural humidity regulators, making buildings more comfortable. However, the standard use of polymer to bind those fibers can be pretty harmful to the environment [1]. In this context, we investigate natural binder such as corn starch as a more sustainable option to bind natural fibers, exploring how this combination cope with heat and moisture transfers in construction materials.

A specific protocol was elaborated for preparing a composite fiber-starch material passing through converting native corn starch into a functional adhesive. Surplus water exceeding 60°C gelatinizes the starch; then, it undergoes drying and grinding cycles to attain a consistent and practicable starch matrix. This matrix is then mixed with natural fibers. Following this protocol, the starch/fibers mass ratio ranges from 0.12 to 0.54, while the medium porosity reaches 70%.

In order to elucidate the mechanisms of water transfers within this material we first focus on the fluid transfers in a starch matrix. Sorption isotherms reveal that starch absorbs a significant moisture content of up to about 30%. Following water transfers during the drying of a starch suspension we show that NMR relaxometry clearly differentiates between two water populations (Fig. 1), with slow exchanges. The first population, labeled as "Free Water", and corresponding to water in pores (i.e., between grains), disappears first and the drying rate remains constant all along this process. The second population, labeled as "Bound Water", and corresponding to water inside starch grains, essentially disappears in a second step (see Figure 1). These characteristics mean that the free water is continuously transported towards the top surface of the sample, even in the ultimate stages of its extraction where this transport likely relies on bound water diffusion. During the second stage of drying, i.e., the extraction of bound water, the bound water is transported by diffusion through the network of contacts between the starch grains. This explains the drying rate decrease during this period (see Figure 1). The validity of this assumption is confirmed by experiments carried out by drying a bound water saturated starch grain packing filled with oil (in the inter-grain porosity). In that case it is shown that bound water is still able to diffuse rapidly (in the solid network) while vapor diffusion through the porosity is precluded. These elements provide fundamental knowledge of water transfers in starch, which will allow to consistently analyze the behavior of the whole composite material.

Based on these experiments, the function of starch as a reactive hygroscopic phase inside a porous medium is confirmed. Our starch is indeed validated as a considerably stable matrix so it can be used as a binder for the natural fibers when formulating bio-composites. Ongoing work aims to refine the processing limits, as well as to characterize the hydric, mechanical and thermal properties of the resulting materials.

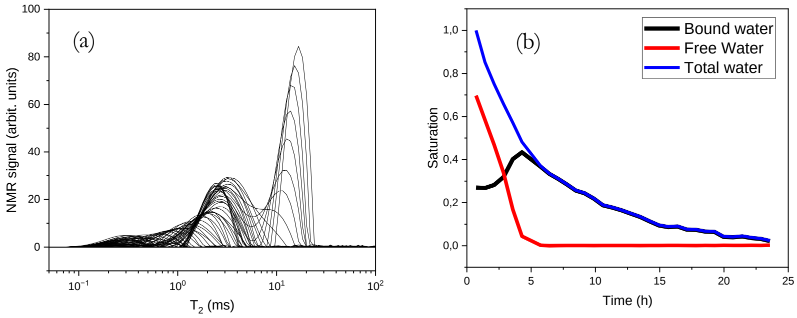

Figure 1: (a) Probability density function (pdf) of the NMR relaxation time at different times during the drying of suspension of native starch with water and (b) water fractions and total water during the drying as extracted from the pdfs.

References

[1] Siouta, L.; Apostolopoulou, M.; Bakolas, A. Natural Fibers in Composite Materials for Sustainable Building: A State-of-the-Art Review on Treated Hemp Fibers and Hurds in Mortars. Sustainability, 16, 10368 (2024)

Water transfers in starch-fibers composites

Olfa HBAIEB[a], Benjamin Maillet[a], Philippe Coussot[a]
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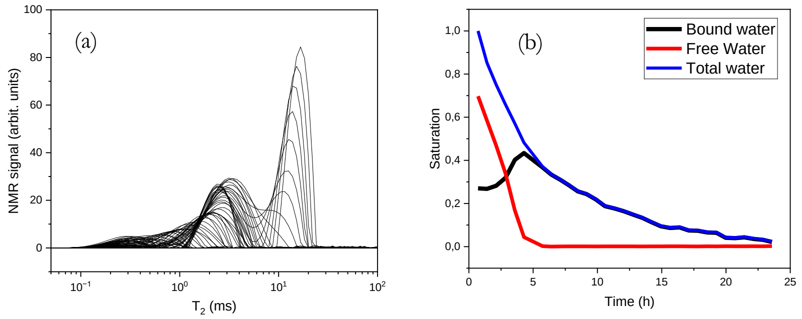

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Incomplete Mixing in Chaotic Flows

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*Keywords: m*ixing, transport, theory, macroscopic model, chaos, fluctuations

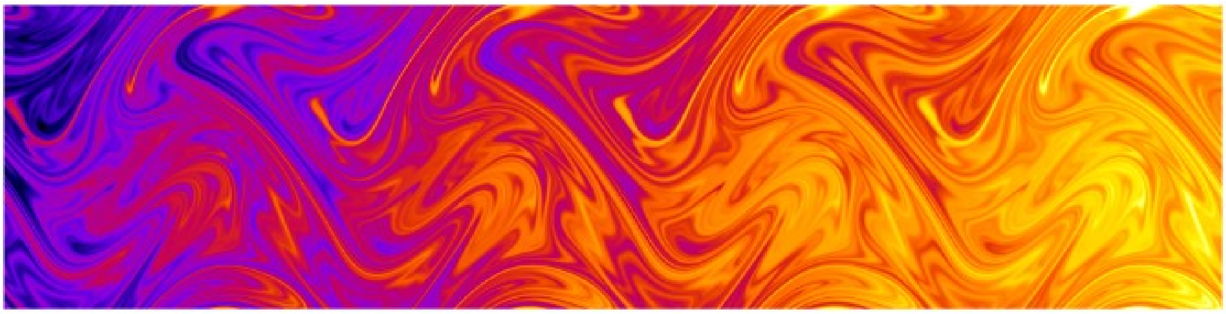

Figure 1: Scalar mixing front formed by a periodically stirred flow producing chaotic advection.

The mixing of fluids is greatly enhanced by the stirring action of a heterogeneous velocity field. Here we investigate the properties of scalar mixing fronts that spontaneously form when mixing two diffusing solute stirred by a smooth chaotic flow. Such flows are commonly found in nature, for instance in laminar flows through porous materials [1,2]. We focus on the statistical distribution of the scalar concentration through the front and the existence of incomplete mixing below the velocity length scale.

To highlight the phenomena, we perform high-resolution direct numerical simulation of advection-diffusion in a time-varying sinusoidal velocity field in the presence of a mean scalar gradient. We show that the shape of the power spectrum density of scalar fluctuations is well captured by the stretching-diffusion evolution model of Kraichnan [3] and that scalar variance inside the front can be entirely predicted from the stretching statistics of the flow field and the molecular diffusion.

Finally, we demonstrate that the evolution of scalar mixing fronts in smooth chaotic flows is well captured through a macrodispersive transport equation for the mean concentrations together with a physically-based closure equation for chaotic microscale fluctuations. This is possible owing to the clear scale separation existing between macroscale dispersive forcing and microscale dissipation in chaotic flows.

These findings open a new avenue to model both conservative and reactive transport in incompletely mixed environments, as it occurs at the pore scale in porous flows.

References

[1] Lester *et* al. Is chaotic advection inherent to porous media flow?, *Phys. Rev. Let.*, *111*(17)174101 (2013).
[2] Heyman et al., Stretching and folding sustain microscale chemical gradients in porous media, *PNAS* 117.24 (2020)
[3] Kraichnan, Convection of a passive scalar by a quasi-uniform random straining field. *Journal of fluid mechanics*, *64*(4), 737-762. (1974).

Scalable flow modeling in karstic media through graph simplification

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Keywords: Karst Networks, Graph Theory,

Karst aquifers are characterized by highly heterogeneous and complex conduit networks, making the modeling of groundwater flows particularly challenging, especially under unsaturated flow conditions. In this work, we model these systems as resistive graphs, where nodes represent junctions and edges simulate hydraulic conductance through karst conduits. The governing equations take the form of nonlinear Laplacian systems and can involve graphs with tens of thousands of nodes. To enable efficient computation and scale transition, we propose a coarsening strategy that simplifies the graph while preserving key global hydraulic properties. Our approach relies on the concept of effective resistance to guide the simplification process, ensuring that the reduced network maintains comparable flow behavior between designated zones. We assess the performance of the coarsened graphs by comparing their flow responses to those of the original fine-scale networks. Preliminary results show that significant reductions in graph size are possible with limited loss in accuracy, providing a promising framework for multi-scale modeling of karst systems. This method paves the way for computationally efficient simulations of large-scale subsurface flow, and for better understanding of flow redistribution in evolving karst architectures. Figure 1 illustrates a subgraph extracted from a complex conduit network and its corresponding coarsened version obtained through our effective resistance-based simplification method.

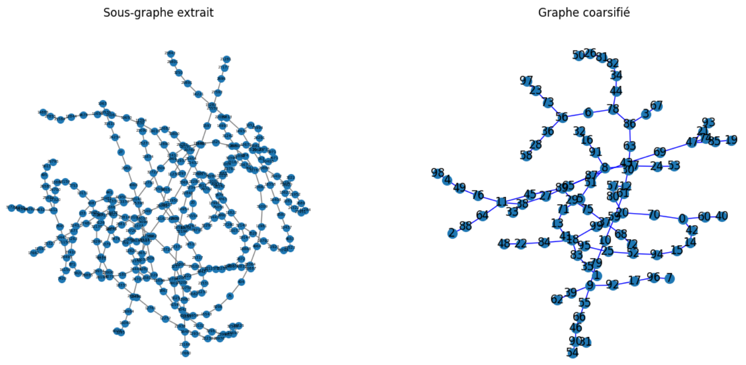

Figure 1: Original and simplified network structures.

References

[1] W.Ellens, F.M. Spieksma, P.Van Mieghem, A.Jamakovic, R.E. Kooij. *Linear Algebra and its Applications 435 (2011) 2491-2506: Effective graph resistance.* ELSEVIER.

[2] Colecchio, I., Le Gall, E., Noetinger, B. (2025). Effective conductivity of conduit networks with random conductivities. arXiv:2503.09457v1 [cond-mat.dis-nn]. https://arxiv.org/abs/2503.09457v1

[3] Collon P., Bernasconi D., Vuilleumier C., Renard P. (2017). Statistical metrics for the characterization of karst network geometry and topology. Geomorphology, 283, 122â142

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Scallop Formation Due To Dissolution-Driven Convection

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Keywords: scallop pattern, mineral dissolution, density-driven flow, micro-continuum modelling, Volume of Solid approach

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When the mineral surface of a soluble rock, such as salt, is immersed in water, it begins to dissolve, leading to the formation of a denser fluid layer near the fluid-solid interface. Due to gravitational forces, the denser layer tends to detach and sink, displacing the lighter fluid, which in turn rises to take its place. This gravitationally unstable motion, coupled with surface dissolution, gradually carves cup-shaped depressions bordered by sharp crests into the surface. These striking morphological features, commonly referred to as scallops, arise from an interplay among fluid flow, chemical reactions, and surface morphology [1]. However, such complex processes have been studied only to a limited extent and remain poorly understood.

In this work, a micro-continuum modelling technique is employed to simulate the scallop formation, considering the solid mineral as a low-permeability porous medium [3]. This hybrid-scale approach effectively captures the displacement of the fluid-solid interface due to mineral dissolution without the need for re-meshing of the computational domain. Surface reactions are localized using an improved Volume of Solid approach, based on the divergence of a reactive flux [2]. This formulation offers enhanced accuracy and does not require a localization function to track the dissolving surface. Fluid-density variations, induced by the concentration gradient of dissolved minerals, are calculated using a linear relationship between density and solutal concentration, and are incorporated under the Boussinesq approximation.

Numerical simulations demonstrate the capability of this approach in reproducing the scallop pattern and its evolution. To gain deeper insights into the pattern formation on the dissolving surface, the effects of gravitational instability and chemical reactions on the dissolution process are analyzed. The numerical results, obtained using the finite volume method within an OpenFOAM-based framework, are verified against asymptotic solutions in a limiting case.

References

[1] M. Chaigne, S. Carpy, M. Massé, J. Derr, S.C. du Pont, M. Berhanu, Emergence of tip singularities in dissolution patterns, Proceedings of the National Academy of Sciences, 120, e2309379120 (2023)

[2] J. Maes, C. Soulaine, H.P. Menke, Improved Volume-of-Solid formulations for micro-continuum simulation of mineral dissolution at the pore-scale, Frontiers in Earth Science, 10, 917931 (2022)

[3] C. Soulaine, Micro-continuum modeling: An hybrid-scale approach for solving coupled processes in porous media, Water Resources Research, 60, e2023WR035908 (2024)

Convective Dissolution of CO_2 in Index-Matched Porous Media: A Shadowgraphy Study

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Keywords: porous media flow, CO_2 convective mixing, variance analysis, shadowgraphy

Long-term carbon-dioxide (CO_2) storage is a key strategy for achieving the goals of the 2015 Paris Agreement [1]. To improve the efficiency and safety of CO_2 storage in saline aquifers, post-injection processes need to be better understood. One critical process is convective dissolution, where CO_2 first diffuses into brine, triggering buoyancy-driven convection thanks to density mismatch. Despite the physicochemical processes being well-characterised, open questions remain about the 3D convective dissolution of CO_2 in porous rocks. This work aims to make use of an experimental method based on shadowgraphy to study CO_2 convection in a transparent, saturated porous medium.

In a recent study, we reported on our first investigation of convective dissolution by shadowgraphy and with miscible analogue fluids in a saturated transparent porous medium [2]. In this follow-up work, we apply the same methods to study the convective dissolution of CO_2 in a saturated porous medium at high pressure and controlled temperature. We investigate Rayleigh numbers (Ra) ranging from 10^3 to 10^4, by varying the CO_2 injection pressure, thus obtaining various density differences. By investigating the temporal evolution of the image variance, we can detect distinct regimes of the CO_2 dissolution process, pure Fickian diffusion, onset of convection in the form of plumes, and fully developed convective mixing. Additionally, we are able to measure the plume speed (Figure 1) and quantify the convective flux, corroborating the findings from our previous study on miscible analogue fluids.

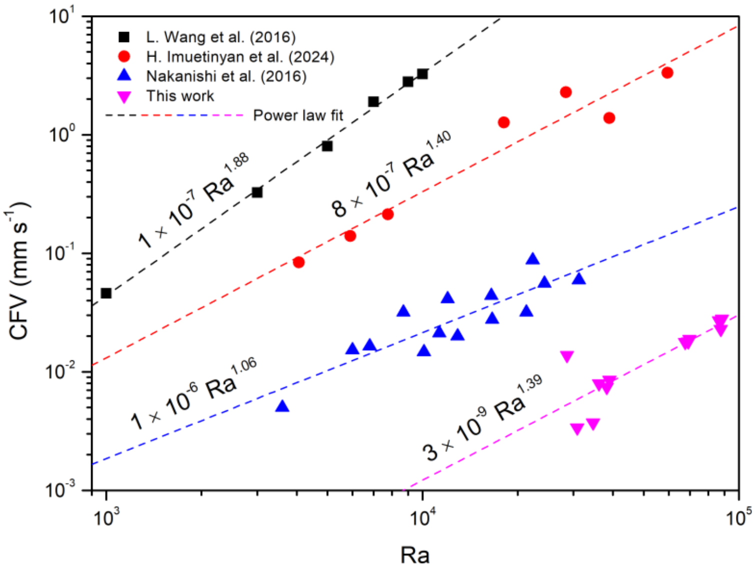

Figure 1: Average convective front velocity (CFV) as a function of Ra for different experiments.

References

[1] Rogelj, J., Geden, O., Cowie, A., Reisinger, A., Net-zero emissions targets are vague: three ways to fix. *Nature* 591, 365–368. (2021).

[2] H. Imuetinyan, P. Fruton, C. Giraudet, and F. Croccolo, "Convective plume spreading in model transparent porous media," *Transport in Porous Media*, pp. 1687–1708, (2024).

Dynamics of Gadolinium Oxide Clogging in Porous Media: Insights from 4D X-ray Microtomography

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[2]Géosciences Environnement Toulouse, Université de Toulouse
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Keywords: Rare earth elements, porous media and flow, pore-clogging, colloidal transport

The mobility of rare earth element (REE) nanoparticles in subsurface environments is a growing concern due to their increasing use and potential ecological risks [1]. The dynamic monitoring at the micro scale of gadolinium (Gd) nanoparticle transport holds significant potential in biomedical and environmental applications, however, the existing literature is scarce and is mostly focused on the macroscale column studies [2],[3]. In this study, we investigate the pore-scale mechanisms governing the transport and retention behavior of Gadolinium oxide (Gd_2O_3) nanoparticles under single-phase flow conditions within porous media using high-resolution 4D X-ray microtomography. Gd_2O_3 was selected as a representative REE nanoparticle due to its high X-ray attenuation, allowing direct visualization of its spatiotemporal distribution in situ. Experiments were conducted using cylindrical sintered glass columns (4 mm diameter, 40 mm length) with pore throat sizes ranging from 40 to 100 µm, which were pre-saturated with 80% glycerol at an ionic strength of 10mM NaCl (figure 1). The influence of flow velocity on nanoparticle retention was systematically analyzed. Our results reveal distinct retention mechanisms, including straining at pore throats and reduction in permeability due to clogging of the pores. These localized depositions, quantified in terms of Gd_2O_3 concentrations, were shown to alter local flow paths, highlighting the coupling between colloid dynamics and hydrodynamic conditions. This study provides new insights into the fate of REE nanoparticles in the subsurface, which is essential for risk assessment and remediation strategies. These experiments will also guide the future surface complexation modeling of REE and numerical modeling simulations of fluid flow and transport.

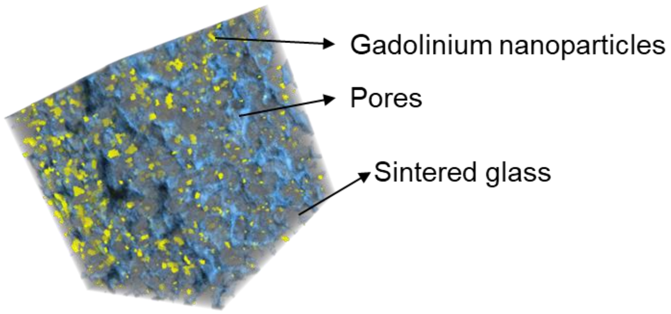

Figure 1 Distribution of Gadolinium nanoparticles through sintered glass porous media.

References

[1] A. Drobniak and M. Mastalerz, "Rare Earth Elements: A brief overview," *Indiana Journal of Earth Sciences*, vol. 4, Jan. 2022, doi: 10.14434/ijes.v4i1.33628.
[2] A. Menahem, "Transport of gadolinium- and arsenic-based pharmaceuticals in saturated soil under various redox conditions," 2016.
[3] M. Iqbal, R. Marsac, M. Davranche, A. Dia, and K. Hanna, "A mechanistic surface complexation approach for the prediction of rare earth element reactive transport in quartz porous media," *Chemical Geology*, vol. 634, p. 121601, 2023, doi: https://doi.org/10.1016/j.chemgeo.2023.121601.

Pore size distribution of Lorraine coal using NMR relaxometry and cryoporometry

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Keywords: Coal; Low field 1H NMR; T2 Relaxation; Cryoporometry; Pore size distribution

This study focuses on characterizing the pore structure of coal samples from the Tritteling borehole (Lorraine region) using two low-field nuclear magnetic resonance techniques, T2 relaxometry and cryoporometry. While conventional methods such as mercury intrusion porosimetry (MIP) and low-pressure adsorption (LPA) are widely used to characterize coal pore structures, the application of non-destructive NMR method remains relatively limited. The use of T2 relaxometry [1] and cryoporometry [2-3] enables an accurate approach to measure the pore size distribution of nanoporous materials. The coal sample (small pieces of coal or coal powder) placed in NMR-tube was first saturated with pure water with given water quantity. From the saturated state, the sample was progressively dried in an oven, and for each drying step, its water content was determined by weighing and T2 relaxation was measured in a low-field NMR spectrometer (Mq20 Bruker). The results show that powdered coal offers more advantage than small pieces for NMR measurements, probably due to better access of water to the smallest pores (micropores and mesopores). Analysis of the T2 relaxation time distributions revealed two main pore-size categories. Water associated with micropores exhibited relatively short T2, ranging from 0.1 to 0.5 ms (corresponding to pore sizes from 0.5 to 3 nm with the surface relaxivity of coal given in the literature), while the one associated with mesopores displayed longer T2, ranging from 0.5 to 66.8 ms (pore sizes from 3 to 400 nm). During the drying process, the T2 peak of the mesopores gradually shifted towards shorter relaxation time referring to the evaporation mechanism within these pores while the peak of micropores remained unchanged at the beginning of drying and slowly disappeared at the end of the process. This result underscores that during drying water desorbs firstly from the mesopores and subsequently from the micropores. In addition, a quantitative relationship between water content and NMR signal for each pore category was established, allowing us to estimate the porosity of the samples. Another NMR technique for measuring pore size distribution was used, namely NMR cryoporometry. This method involves progressively melting the initially frozen water at a very low temperature inside the pores of the porous medium, the phase change temperature being shifted due to confinement according to the Gibbs-Thomson law. Coal samples (pieces and powder) were progressively warmed from -45℃ to +5℃, and NMR-T2 measurements, conventionally obtained by the CPMG sequence were carried out at different temperature levels. This technique makes it possible to measure the characteristics of increasing spin echo signals of water during the phase transition, as ice inside the pores progressively melts into liquid water. By measuring the amount of NMR signal as a function of temperature, the pore size distribution can be reconstructed directly. Finally, by combining the two approaches, it is possible to verify and refine the characterization of the pore structures. More generally, this approach highlights the potential of combining T2-NMR relaxometry and NMR-cryoporometry techniques to assess the surface relaxivity of nano-porous materials and obtain their pore size distribution in greater detail and accuracy.

References

[1] Y. Yao, D. Liu, Y. Che, D. Tang, S. Tang, W. Huang, Petrophysical characterization of coals by low-field nuclear magnetic resonance (NMR), Fuel 89 (2010).
[2] J.H. Strange, M. Rahman, E.G. Smith, Characterization of porous solids by NMR. Phys. Rev. Lett., 71-21 (1993).
[3] J. Mitchell, J. B.W. Webber, J.H. Strange, Nuclear magnetic resonance cryoporometry, Phys. Rep. 461 (2008).

Impact Of Sedimentary And Diagenetic Heterogeneities On Petrophysical Properties (Φ, K, P wave) Of Continental Limestones

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Keywords: Continental limestone, Porosity, Permeability, P-wave velocity, Diagenetic facies

The internal structure of sedimentary rocks, such as limestones, is governed by sedimentary, diagenetic, and tectonic processes. In the case of groundwater management, it is required for estimating the quantity and quality of groundwater, as well as for understanding the nature of heat and mass transfers occurring within it. The size and architecture of pores, fractures, and potential karst networks result from the evolution of a primary sedimentary facies into a secondary diagenetic facies. Consequently, the petrophysical properties of limestones evolve based on the initial sedimentary facies, potential fluid flows, temperature, pressure, geochemical conditions, or tectonic events.

A heterogeneous primary limestone, such as **continental lacustrine and palustrine limestone**, leads to varying levels of diagenesis, resulting in diverse secondary facies, distinct petrophysical properties at different scales and therefore requires further studies to be linked with geological and geophysical data [1]. Our study focuses on the observatory of the vadose zone ("Observatoire des transferts dans la Zone Non-Saturée", O-ZNS) near Orleans, which aims to better understand fluid and heat transfers throughout the complex **Beauce Limestones formation (Aquitanian continental limestones)**. The 20-meter-deep and 4-meter-wide artificial well, along with various drilled and logged boreholes, provides an exceptional quantity of data and samples for investigation.

Through this contribution, we seek to decipher the link between the petrophysical properties of heterogeneous continental limestones and their sedimentary and diagenetic facies at the centimetre scale and below. The primary properties investigated in this study are **P-wave velocity**, **porosity**, and **permeability** at **various saturation levels**. The results of these measurements will be compared with **thin-section observations** to attempt elucidating the relationship between diagenesis and physical properties. Additionally, we will compare these properties across different levels of diagenesis to build representative geological, hydrogeological and geophysical logs.

These measurements, conducted on **16 primary sedimentary facies**, allow us to group certain facies into **diagenetic facies** with similar physical properties, highlighting the influence of diagenesis on petrophysical characteristics. Conversely, we can identify distinct diagenetic facies within a single sedimentary facies, further emphasizing the impact of diagenetic processes on the evolution of these properties.

References

[1] M. Abbas, J. Deparis, A. Isch, C. Mallet, C. Jodry, M. Azaroual, B. Abbar, J.M. Baltassat. Hydrogeophysical characterization and determination of petrophysical parameters by integrating geophysical and hydrogeological data at the limestone vadose zone of the Beauce aquifer. Journal of Hydrology. https://doi.org/10.1016/j.jhydrol.2022.128725

Intrinsic permeability of heterogeneous porous media

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Abstract

Providing a sound understanding of the relationship between flow (Q) and pressure drop(ΔP) for porous media is a long-standing fundamental research challenge. A wide variety of environmental, societal and industrial issues, ranging, e.g., from water-soil system remediation to subsurface energy optimization, is affected by this critical issue. While such dependence is well represented by the Kozeny-Carman formulation for homogeneous media, the fundamental nature of such a relationship (Q vs ΔP) within heterogeneous porous systems characterized by a broad range of pore sizes is still not fully understood. We design a set of controlled and complex porous structures and quantify their intrinsic permeability through detailed high quality microfluidics experiments. We rationalise the results linking the overall intrinsic permeability to the microscopic features of the porous structure. Our formulation explicitly embeds the spatial variability of pore sizes into the medium permeability through a conceptualization of the system as a collection of smaller scale porous media arranged in series. The resulting analytical formulation yields permeability values matching their experimentally-based counterparts without the need of additional tunable parameters. Furthermore, in addition to advancing the theoretical understanding of this important relationship, we extend our framework by incorporating novel experiments on biofilm growth, specifically investigating the spatiotemporal distribution of growth for motile and non-motile bacterial strains, which influence the system permeability by obstructing pore spaces.

Iterative Coupling Algorithms For Mixed-Dimensionnal Poromechanical Models In Faulted Geological Systems

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Keywords: Iterative coupling, Anderson acceleration, Fractured/faulted models

Coupled poromechanical models are essential for understanding and managing risks in geoscience applications like geothermal energy and CO_2 sequestration, where fault reactivation can lead to leakage or induced seismicity. These models simulate complex interactions between multiphase fluid flow, rock deformation, and fault mechanics. Their numerical implementation is challenging due to geological heterogeneity, complex geometries, and strong multiphysics couplings.

Three main numerical approaches exist:

1. Monolithic (Newton-based) methods solve all equations simultaneously but lack modularity, are computationally intensive, and require advanced preconditioners.
2. Time-splitting methods [1, 2] decouple fluid flow and mechanical sub-models, allowing smaller time steps for flow but may lose accuracy and robustness under strong coupling or regime shifts.
3. Iterative splitting methods offer a balanced solution by iteratively solving sub-models until convergence. They are more modular, support sub-time steps, and can be enhanced with acceleration techniques like Newton-Krylov, Conjugate Gradient, or Anderson methods to improve robustness and efficiency.

In our work, we focus on iterative splitting methods due to their modularity and flexibility. We observe that the resulting fixed-point algorithm performs well in scenarios without fracture slip. However, when slip initiates in the fracture, the algorithm either fails to converge or converges very slowly. To address this limitation, we have successfully applied Anderson acceleration [3] to the iterative splitting approach. This enhancement significantly improves robustness—enabling convergence even when fracture slip occurs—and also increases computational efficiency by accelerating the convergence of the fixed-point iterations.

References

[1] T. Almani, K. Kumar, Convergence of single rate and multirate undrained split iterative schemes for a fractured Biot model, Computational Geosciences, 6, pp. 975-994, 2022.
[2] V. Girault, K. Kumar, and M. F. Wheeler. Convergence of iterative coupling of geomechanics with flow in a fractured poroelastic medium. Computational Geosciences, 20 (5), 997–101, 2016.
[3] J. W. Both, K. Kumar, J. M. Nordbotten, F. A. Radu, Anderson accelerated fixed-stress splitting schemes for consolidation of unsaturated porous media, Computers & Mathematics with Applications 77 (6) (2019) 1479 – 1502.

Experimental Investigation of Salt Precipitation in Rock Samples for Hydrogen Storage Applications

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Keywords: Salt precipitation, underground hydrogen storage, microcomputed tomography

The severity of climate change brings serious challenges that demand substantial efforts to accelerate the transition to low-carbon energy systems. One promising approach is utilizing porous geological formations, such as saline aquifers and depleted reservoirs, for hydrogen storage to balance out the fluctuating nature of renewable energy sources. However, the distinct chemical and thermodynamic properties of hydrogen introduce complexities which can impact operational efficiency and safety. One of the underexplored issues in underground hydrogen storage is the risk of salt precipitation during injection, arising from the evaporation of saline water present in the porous formations. While the risk of injectivity impairment due to the salt precipitation is well known from field cases and related research on other underground stored gases, such as CO_2 [1], hydrogen's unique properties may alter dry-out behaviour and precipitation dynamics. Therefore, pore-scale observations of salt precipitation during hydrogen injection are important for accurately evaluating this risk factor specific to the hydrogen storage case. To address this, we performed in situ flow experiments under reservoir conditions (65°C, 50 bar) on Bentheimer sandstone. Using micro-CT imaging, we monitored the evolution of dry-out while maintaining a constant hydrogen injection rate for brines with two different salts: potassium iodide and sodium chloride. We found that the accumulation rate and behaviour of supersaturated brine (or salt) on the injection surface differed depending on the salt type. However, in both cases, we observed a redistribution of the supersaturated brine (or salt) from the injection surface towards the inner pore space at the later stages of the dry-out. This significantly altered the spatial distribution of salt at the end state, ultimately reducing porosity by 10%. We used a single-phase flow solver (poreFoam [2]) to obtain the gas relative permeability of the final state and estimated a 35% relative permeability reduction due to dry out. Our results suggest that the main mechanisms contributing to salt precipitation remain similar to those observed when nitrogen is used as a surrogate gas [3]. However, the newly observed salt redistribution within the sample needs further investigation, as it directly impacts injectivity impairment.

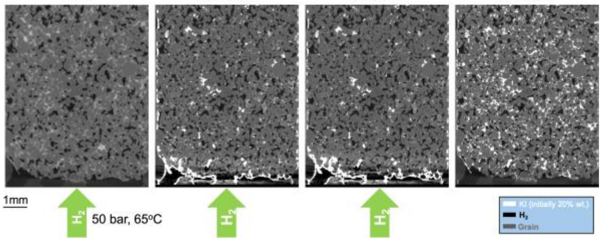

Figure 1: Temporal evolution of salt precipitation and redistribution in the pore space.

References

[1] Baumann, G., Henninges, J., De Lucia, M., Monitoring of saturation changes and salt precipitation during CO2 injection using pulsed neutron-gamma logging at the Ketzin pilot site, International Journal of Greenhouse Gas Control, 28, 134-146 (2014).
[2] Raeini, A.Q., Blunt, M.J. and Bijeljic B., Modelling two-phase flow in porous media at the pore scale using the volume-of-fluid method, *Journal of Computational Physics*, 231, 5653-5668 (2012).
[3] Kalyoncu Pakkaner, G., Cnudde, V., Derluyn, H., and Bultreys, T., Impact of efflorescence on internal salt precipitation dynamics during injection of gases in porous rocks, *Advances in Water Resources*, 201, 104984 (2025).

Impact Of Transient Flow On Reactive Fronts In Porous Media

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Keywords: Reactive Transport, Transient Flow, Hydrodynamic Dispersion, Flow Shear

Groundwater flow is subject to transients, due to natural events or human activities (recharge, tides, decontamination, etc.). The occurrence of such temporal fluctuations in the flow field can have significant impact on reactive transport processes, compared to steady flow conditions, especially in reactive fronts. These fronts manifest as localized interfacial regions where chemical reaction occurs in an ambient flow field that brings two or more reactants in contact with each other. Understanding how reaction fronts evolve during transient flows is therefore key to predicting reactive transport in the subsurface.

In these fronts, reaction rates often depend on the local mixing state of the reactants, which in turn is controlled by the interplay between advective and diffusive processes. Under steady flow conditions, the presence of heterogeneity in the permeability fields has been shown to enhance mixing and reaction at the Darcy scale, due to stretching-enhanced mixing. In contrast, it is currently unknown how transient flows would impact reaction rates.

Here, we conduct reactive transport experiments with transient flow in both Hele-Shaw and index-matched porous media cells. A steady mixing front is created inside the cell by two opposing injection points, creating of a stagnation point flow. Transient flow is then imposed by varying the ratio of the injection rates, causing a displacement of the stagnation point and the mixing front. A bimolecular chemiluminescent reaction is used to quantify the effective reaction rate within the mixing front at all times. We observe that transient flows increase reactivity compared to steady state conditions, both in the local maximum of reaction rates and in the size of the reactive front.

In the Hele-Shaw cell, the enhancement can be up to 3 times compared to steady conditions. The evolution of the reaction front to the new steady state occurs in a time much shorter than that required for Taylor-Aris dispersion, indicating that the reaction front remains in the ballistic shear regime when the reactivity enhancement is observed. Using the lamellar theory for sheared fronts, we find that the maximum reaction rate should scale with the transient flow strength to the power of 3/4, a prediction that compares well with the experimental observations (0.76±0.03).

In the porous media cell, we also observe a power law scaling between the reaction rate enhancement and the transient flow magnitude, with an exponent of 0.58±0.01. In contrast to the Hele-Shaw case, we argue that the mixing enhancement is due to longitudinal hydrodynamic dispersion. Solving the advection-dispersion-reaction equation for the reaction front near the stagnation point yields a theoretical exponent of 1/2, which agrees well with experimental observations.

These results indicate that an important part of the biogeochemical activity in the subsurface can occur during transient events. The proposed modeling framework provides a quantitative prediction of such reactive transport dynamics.

Determination of the Relative Permeability of Earthen Material During Drying Using Magnetic Resonance Imaging

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Keywords: Earthen Material, Relative Permeability, Magnetic Resonance Imaging, Instantaneous Profile Method

Relative permeability is a key parameter governing water flow in unsaturated soils. This study investigates the relative permeability of earthen materials using the Instantaneous Profile Method based on Darcy's law. The method requires the quantification of two primary parameters: water flux and pressure gradient. We determine the water flux by monitoring the spa-tial and temporal evolution of water content during drying, using Magnetic Resonance Imaging (MRI). Then, we calibrate the MRI signal to quantify the water content in each axial slice of the sample. The hydraulic gradient is obtained from the Soil Water Characteristic Curve (SWCC), established over the full range of water contents using a combination of the Hyprop (double tensiometer method) and the WP4 (dew-point Water Potentiometer) apparatuses. By integrating MRI-derived water content profiles with the corresponding matric potential data and applying Darcy's law, we construct relative permeability curves at different positions within the sample. This approach provides detailed insights into the hydraulic behavior of earthen materials under unsaturated conditions.

Intercooler, Porous media, CFD, maldistribution

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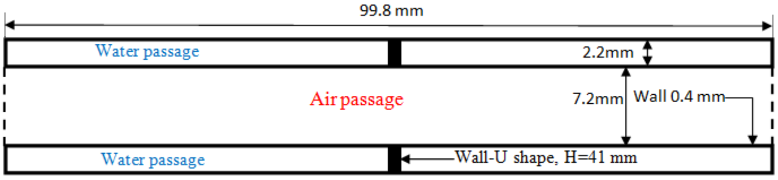
Keywords: Intercooler, Porous media, CFD, maldistribution

Abstract

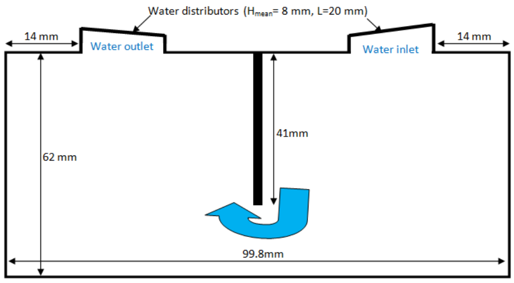
Air intake temperature has significant effects on engine's performance characteristics; exhaust emissions control and reduction, combustion efficiency increase, stability and lower BSFC or fuel economy. Several devices used to regulate the temperature of air entering the engine's intake systems; dynamic device for air transfer (DDAT), integrated thermal deflector (ITD) or advanced thermal protection using new kind of insulated materials. For turbocharged engines, intercoolers are the essential device used to cool charging air. In this study, the coupling of porous media modelling and CFD simulation is used to evaluate the performance characteristics of this king of heat exchanger, namely; the pressure drop and the thermal efficiency. Application of porous media models in internal combustion engines attracted great interest. In this study, it is used to model the water and airflows through the intercooler core because of its complex geometry. In addition, CFD, as one of the most dynamically improved research field is used to simulate the airflow through the intercooler and engine distributors.

1 Model description

Bulkhead or wall in the water passage to force a U-shaped pass and avoid direct passage of water from the inlet to the outlet. Water follows the path represented by the blue arrow in the water passage. Water passages between each air passage tube. Presence of a wall in the center of these water passages (see figure. 01, below).



a) Top view



b) Side view-water passage

Figure 1: Intercooler core model

2 Numerical procedure

2.1 Geometry and mesh generation

The intercooler used is divided into three parts; intercooler distributor, intercooler core and the engine distributor. The 3D model of the intercooler is discretized using a mesh of up to 4167605 of tetrahedral elements.

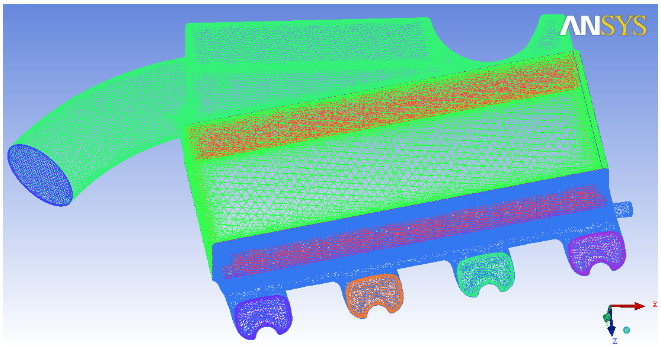


Figure 2: Geometry with mesh generation

2.2 Methodology

Numerical simulation using a porous media model is based on the simultaneous use of Darcy's law to determine the pressure drop and the generalized Navier-Stokes equations. In our case, this model applies only to the core of the exchanger, which contains the air-side and water-side exchange surfaces. The other two parts, the upper casing (intercooler distributor) and the lower casing (engine distributor), are considered as fluid domains.

Thermal efficiency is evaluated as the mass flow averaged temperature of the gases leaving the heat exchanger, To, and pressure drop is evaluated as the pressure differential between outlet and inlet of the heat exchanger, Δp.

The heat exchanger was designed to remove 40.69 Kw from 800 kg/h at 220 °C using 18 liter/min of water at 10.2 °C. Table 1, summaries the necessary given parameters.

	Cold side (water)	Hot side (air)
Flow rate	18 liter/min	800 kg/h
Inlet temperature	10.2^{o} C	220^{o} C
Outlet temperature	42,6	
Inlet pressure	1481.6 mbar	
Pressure drop	241,0 mbar	
Flow arrangement	Cross flow	
Requested heat rejection	40,69 kW	
Effectiveness	95.1%	

The reference pressure (p0) was set to 101325 Pa, from which the inlet pressure values (pinlet, i) have been calculated.

In order to determine the parameters relating to Darcy's law, several numerical simulations have been run to calculate the pressure drop (ΔP) through the porous medium as a function of the filtration velocities at the inlet to this medium, this is achieved by varying the outlet flow rate values (500, 600, 700, 800, 900, 1000 and 1100) kg/h. The porous medium parameters (permeability and quadratic coefficient due to inertial effects) are determined from the relationship (ΔP=13.18912 v+ 1.55312 v2, see graph below) and this is by identification with Darcy's modified law:

$$S_{M,i} = -\frac{\mu}{K_{perm}} U_i - K_{loss}\frac{\rho}{2}|\boldsymbol{U}|U_i \tag{1}$$

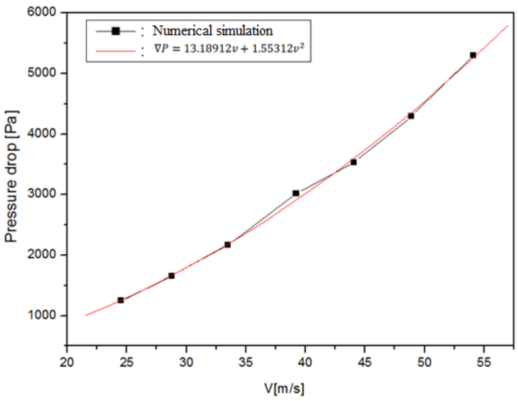


Figure 3: Validation pressure

Isotropic pressure losses due to viscous and inertial effects, applied to porous regions, can be formulated using the permeability coefficient (K_{perm}) and the quadratic loss coefficient from relationship (1). The linear component of this relationship represents viscous losses and the quadratic term represents inertial losses. This part of the momentum equation source term is also, known as Darcy's modified law. By identifying the terms between this relationship and the numerically determined one representing head loss as a function of velocity ($\Delta P = 13.18912\ v + 1.55312 v^2$), we can calculate the permeability coefficient K_{perm} and the quadratic loss coefficient K_{loss}. These are essential for calculations using a porous media models. Alternatively, linear and quadratic resistance coefficients can be used: $C_{R1} = \mu / K_{perm}$ and $C_{R2} = K_{loss}(\rho/2)$.

Stabilizing Emulsions with Surfactant-Nanomaterial Systems in Carbonated Water Injection for EOR

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Keywords: Carbonated water injection, Chemical-based emulsion, Enhanced Oil Recovery

Carbonated water injection has been introduced as a promising method to overcome challenges pertinent to CO_2 injection, such as low sweep efficiency and early gas breakthrough in contact with heavy oil [1,2]. Moreover, chemical reactions in the reservoir with polar components of oil will generate emulsions [2]. Although chemical-based emulsions have been widely studied, their stability under carbonated water injection boosted with chemicals and their influence on EOR and CO_2 storage are not clear. Therefore, the primary objective of this study is to conduct experimental studies that simulate carbonated water injection conditions while varying the pH. Moreover, a series of core flooding and laboratory-scale experiments were performed on a Berea sandstone core with a permeability of 624 mD. Alpha-Olefin Sulfonate (AOS) surfactant was employed at concentration ranges of 1000, 2000, and 3000 ppm, while three types of nanoparticles-silica (SiO_2), zinc oxide (ZnO), and iron oxide (Fe_3O_4)-were introduced at concentrations ranging from 0.05 to 0.3 wt.%, selected. Emulsion stability was systematically evaluated using stability index measurements, rheological analysis, and microscopic droplet size distribution. The addition of nanoparticles significantly improved emulsion stability by reducing droplet coalescence and enhancing viscosity control. Core flooding tests further confirmed the generation of stable in-situ emulsions within the porous medium, resulting in incremental oil recovery beyond that obtained from conventional standalone injection methods. These findings establish that chemical-assisted carbonated water hybrid systems, which enhance emulsion performance and maximize oil recovery under sandstone reservoir conditions and partial CO_2 storage, represent a promising EOR strategy and CO_2 storage.

References

[1] Golkari A, Riazi M. Comparative study of oil spreading characteristics for water and carbonated water systems using live and dead oils. J Pet Sci Eng 2018;171:242–52. https://doi.org/10.1016/j.petrol.2018.07.034.

[2] Salehpour M, Riazi M, Malayeri MR, Seyyedi M. CO2-saturated brine injection into heavy oil carbonate reservoirs: Investigation of enhanced oil recovery and carbon storage. J Pet Sci Eng 2020;195. https://doi.org/10.1016/j.petrol.2020.107663.

Characterization of Porous Metallic Structures Made by Additive Manufacturing for Heat Pipe Applications

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Keywords: Heat Pipes, Capillary Performances, Laser Powder Bed Fusion

Heat pipes are highly efficient heat transfer devices based on the phase change of a fluid, enabling large quantities of energy to be dissipated. Their performance is highly dependent on the internal structure of the capillary wick, which must ensure a compromise between capillary pumping and permeability. However, conventional technologies (grooving, mesh and sintering) present limitations in terms of porosity control and pore distribution.

This work explores the use of Laser Powder Bed Fusion (LPBF) to design innovative porous AlSi10Mg structures. This layer-by-layer process enables the generation of porous networks controlled either by specific designs (determinist approach [1]), or by adjusting the printing parameters inducing a controlled amount of “lack of fusion” pores (stochastic approach [2]), or by a hybridization of both approaches

Several samples were manufactured to understand the relationship between process parameters and capillary properties. To compare the performance of the various specimens, two experiments were performed: a capillary rate-of-rise (ROR) experiment (Figures 1a & 1c) and a fluid-forced flow one. The hybridization approach leads to an overall better performance.

3D images of samples were obtained by micro-computed tomography (µCT) (Figure 1b) and allowed numerical simulations of the permeability on 3D volumes, enabling the understanding of local phenomena. The final goal is to optimize wick design and, ultimately, integrate these structures into functional heat pipes.

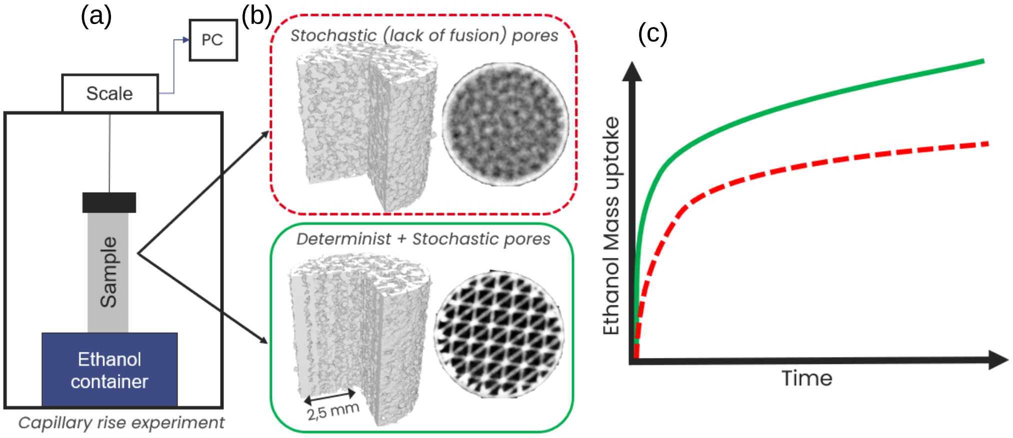

Figure 1: (a) Porous sample in the ROR bench; (b) µCT images and (c) ROR curves of two different porous structures

References

[1] Davoud Jafari, Metal 3D-printed wick structures for heat pipe application: Capillary performance analysis, *Applied Thermal Engineering*, Volume 143, Pages 403-414 (2018)

[2] Cameron Noe, Structured, sintered, and rastered strategies for fluid wicking in additively manufactured heat pipes, *Additive Manufacturing*, Volume 99, 104669 (2025)

Streaming Potential Simulation in Variably Saturated Fractured Porous Media

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Keywords: fractures, mixed hybrid finite element, streaming potential, variably saturated porous media

Electrical Geophysics tools are recognized as practical and non-destructive for investigation of porous media and their characteristics. Streaming Potential (SP) is a passive geophysical tool that has the ability to estimate certain parameters associated with fluid flow in porous media. The charge mobility can be linked to electrical conductivity, fluid content and flow. This link forms the basis for SP measurements. With the addition of information about the pressure boundary conditions, SP data can be used to estimate the permeability. Moreover, increasing the available data and using a robust inversion/treatment techniques can help us locate sharp heterogeneity (e.g. conduits or fractured zones). However, this can only be done if the forward model used in the process of inversion is capable of simulating fluid flow and electrical charge distribution in variably saturated fractured media, a highly nonlinear coupled problem, accurately and efficiently. In addition numerical modelling of SP is of high interest to purposes such as sensitivity analyses and parameter estimation.

We have developed a model based on the combination of hybrid dimension (i.e. fractures considered as lower dimension entities) discrete fracture/matrix approach for discretization of the Richard's equation and the streaming potential using a combination of the mixed hybrid finite element method (i.e. for spatial discretization) and the method of lines (i.e. for the temporal integration). The results have been validated with an equi-dimensional discretization of the same system using COMSOL Multiphysics® (Figs. 1b and 1c). Certain responses in regards to properties associated with the geometry and hydro-dynamic properties of the fracture have been simulated and studied. The results show that the geometrical and hydro-dynamical properties of the fracture can change the electrical response measured compared to that of a non-fractured sample, suggesting the application of SP in the detection of conduits in unsaturated media.

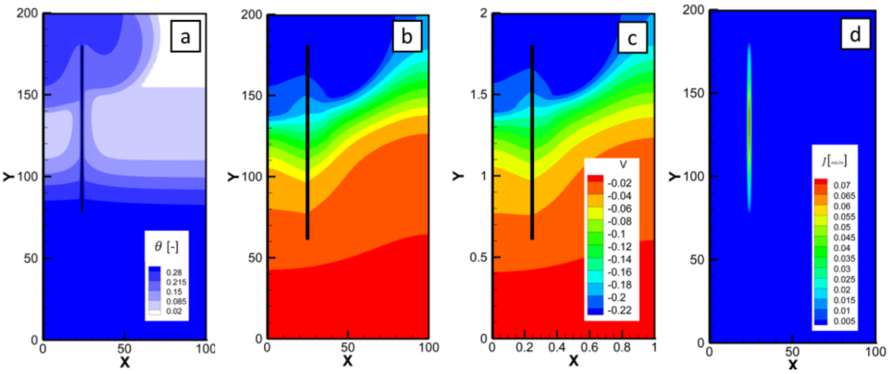

Figure 1: (a) the water content after one hour of injection, (b) the hybrid dimension results of SP simulation, (c) the equi-dimensional results of SP simulation and (d) current density

A double medium approach for modelling seawater intrusion in fractured aquifers

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Keywords: double medium, fractured porous media, seawater Intrusion, variable density flow

Seawater intrusion is the process of saltwater intrusion into coastal freshwater aquifers. Seawater intrusion is a source of freshwater contamination that can affect the lives of millions of people. Coastal aquifers are increasingly vulnerable to seawater intrusion due to increasing anthropogenic activities and climate change. Extensive research has been conducted on numerical modeling of this process. The Variable Density Flow (VDF) model, which takes into account the mixing zone and salinity gradients, is currently the most realistic approach to capture the dynamics of seawater intrusion. However, the VDF model is complex and computationally demanding due to the high nonlinearity and interrelationship of flow and transport mechanisms. This complexity is further increased when fracture networks are present in coastal aquifers. Modeling seawater intrusion in fractured coastal aquifers requires robust modeling approaches that balance accuracy and computational efficiency for a desired scale. Existing modeling strategies include the continuum model, dual or multiple continuum models, discrete fracture models (DFM), and combined discrete-continuum approaches. Each has strengths and limitations with respect to computational requirements, accuracy, and applicability to different scales.

We have developed a novel computationally efficient and flexible numerical model for simulating seawater intrusion in fractured coastal aquifers by coupling the double medium (DM) approach with the VDF model. The DM model conceptualizes the aquifer as two media composed of fractures and porous matrix, with mass and momentum exchange between them represented by coupled continuity/Darcy equations and mass transport in mobile (i.e., fractures) and immobile (i.e., matrix) media. The newly developed model uses advanced numerical techniques for both spatial and temporal discretization. Specifically, it employs a hybrid mixed finite element method for flow simulation and a combination of discontinuous Galerkin methods and multipoint flux approximation for solving the transport equations. These methods improve computational efficiency while maintaining high accuracy.

The developed model is validated for the famous Henry problem, a well-known benchmark for seawater intrusion. Different scenarios and configurations are simulated and the effect of certain parameters (i.e., in particular, the momentum exchange parameter and the salt exchange parameter) is studied. A simplified parameter estimation is then performed to extract values for the salt exchange parameter by comparing the results of the DM model with those of a DFM. By considering the fracture configurations and salt water exchange dynamics, this research contributes to a more efficient and scalable modeling framework for water resources management in coastal regions. It is suggested that this model can form the basis for other tools for different applications (i.e. geothermal and/or electrical geophysics) in natural and artificial fractured porous media. In addition, we believe that considering that the model uses the mixed hybrid finite element method, known for its ability to handle highly heterogeneous domains and its high performance efficiency, it can be the perfect forward module for gradient-based inverse models.

Skin factor model for CO_2 injection in coalbed reservoir

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Keywords: CO_2 storage in CBM, Well Index, Skin Factor, Poromechanics

The coalbed methane reservoir referring to an unconventional reservoir presents a specific geologic formation composed of a natural fracture networks (cleats) of low permeability and coal seam matrix characterized by abundant adsorption sites for gas. The latter offers a huge potential of gas storage within the nanopores with a pore size typically of several nanometers. CO_2 storage in the coal seam consists in using preferential adsorption of CO_2 compared to other gases. When injecting CO_2 into coal reservoirs, CO_2 is adsorbed at the adsorption sites within the coal matrix and the coalbed methane is released and recovered as free gas. On the one hand, CO_2 remains stored within the coal seam and on the other hand, this procedure enhances the methane production as more CH_4 can be desorbed from the nanopores due to high adsorption potential of CO_2.

In this work, we introduce a novel skin factor model to quantify the deterioration of the injectivity index during injection of CO_2 for sequestration in coalbed methane reservoir, accounting for geomechanical coupling effects. The deterioration arises from cleat closure due to pore pressure buildup, which reduces gas adsorption and the solvation force in the nanopores in the coal matrix [1, 2]. Consequently, the matrix swells, leading to a decrease in cleat permeability and, ultimately, a reduction in injectivity. The proposed skin factor formulation is derived from a three-scale model that integrates pore-scale interactions, mesoscale flow and mechanics, and field-scale effects. At the nanoscale, the solvation force is computed using Density Functional Theory (DFT) [3] to describe molecular interactions affecting adsorption and swelling. At the mesoscale, fluid flow and geomechanical deformation are coupled through the Barton-Bandis law, which governs cleat deformation under stress. The hydromechanical system is pre-solved in a preprocessing step to compute the injectivity index and skin factor for the coarse-grid cells intersecting the injection well.

Numerical simulations demonstrate the impact of injectivity deterioration on the efficiency of CO2 storage, highlighting how geomechanical effects influence long-term sequestration potential. Our findings underscore the importance of incorporating coupled hydromechanical modeling in the assessment and optimization of CO2 injection strategies in coalbed methane reservoirs.

References

[1] Q. D. Ha et al., Upscaling poromechanical models of coalbed methane reservoir incorporating the interplay between non-linear cleat deformation and solvation forces, International Journal of Solids and Structures, 262-263, 112083- (2023).

[2] T. D. Le et al, Multiscale model for flow and transport in CO2-enhanced coalbed methane recovery incorporating gas mixture adsorption effects, Advances in Water Resources, volume 144, 103706- (2020).

[3] Q. D. Ha et al, Solvation force and adsorption isotherm of a fluid mixture in nanopores of complex geometry based on Fundamental Measure Theory, Journal of Physics: Condensed Matter, volume 33, 335002- (2021).

Insights Into Bangham's Law With Molecular Simulations: Surface Stress vs. Surface Tension in C-S-H

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Keywords: sorption-induced deformations, Bangham effect, surface stress, molecular simulations

Bangham's law is used to predict the deformation of porous bodies due to fluid adsorption (e.g., for coal in the presence of CO_2 or a wet body upon its drying): this law relates those deformations to the variations of the surface tension of the surface of the pores consecutive to the sorption processes. However, subsequent thermodynamic reasoning has demonstrated that deformations are due to variations of surface stress and not surface tension: Shuttleworth equation shows that surface tension and surface stress are two different –but related– thermodynamic quantities. Nevertheless, a more detailed understanding of the difference between these two entities and their variations with sorption remains essential, especially because the surface stress is difficult to measure experimentally.

To gain new insight into this question, we use molecular simulations to investigate surface stress, tension, and water sorption in calcium silicate hydrates (C-S-H), which are the glue of cement-based materials. First, we perform Grand Canonical Monte Carlo (GCMC) simulations of water in two C-S-H slit mesopores that differ by their Ca/Si ratio (and are equal to 1.1 or 1.7) and obtain water adsorption isotherms at 6 temperatures ranging from 300 K to 525 K. Second, at given amounts of water in micropores (corresponding to given relative humidities), we simulate closed and open mesopores: the pressure difference between the two configurations provides a value for the surface stress at the various water contents. The results show that the surface stress of the C-S-H surface is on the order of several hundred mN/m. Comparing this surface stress and the surface tension calculated with the Gibbs adsorption isotherm, we show that the magnitudes of the variations of the surface stress and surface tension of the C-S-H surface with water adsorption differ from each other significantly.

Evolution of cohesive contact surface area in biocemented granular media characterized by X-Ray µ-tomography

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Bio-calcification, dissolution, X-ray µ-tomography, reactive flow

The microbially induced calcite precipitation is a reinforcement technique that uses the bacteria activity to turn sand into a cohesive medium, inducing the precipitation of calcite crystals in the pores that bond grains together [1]. One of the challenges for its industrial spreading is characterizing the durability of this reinforcement and in particular, predicting how the mechanical behaviour of a biocemented media evolves in an acidic environment (acid rain, industrial pollution…). Indeed, initial work performed by our group has shown that exposing a biocalcified material to an acidic solution rapidly reduces the strength of this material [2].

To understand better the interactions between transport, chemistry, and mechanics, this study have been complemented by in-situ X-ray tomography dissolution experiments at Ghent University and at a synchrotron facility (Soleil). Dissolution of biocemented granular media was performed under different flow rates and pH in order to understand the temporal and spatial evolution of the calcite distribution within the medium, with a special interest in the evolution of the cohesive contact surface area that creates the cohesion.

First observations (Figure 1) show that preferential pathways along which calcite rapidly dissolves, appear when the flow rate is high and the pH is low, whereas a flat dissolution front forms when the flow rate is low and the pH is close to seven. Once the evolution of the cohesive contact area will be extracted, they will be used as input parameter in a Discrete Element Model we have developed [3] in order to predict the evolution of the strength of the material.

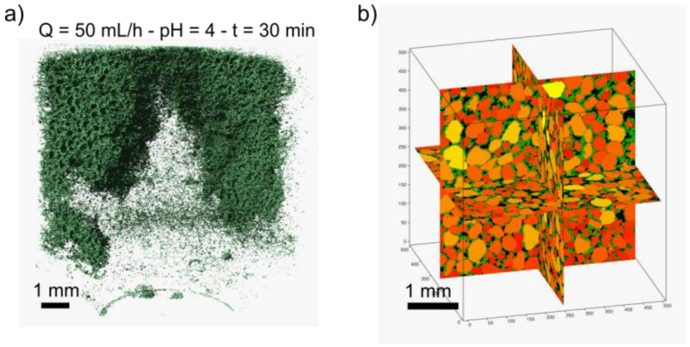

Figure 1: a) Segmented cross sections of a biocemented granular column (green: calcite, black: porosity, hot color map : sand). The color map represents the cohesive contact surface area of each grain. b) 3D image of the calcite (sand removed) after 30 min of dissolution.

References

[1] J. T. DeJong, et al., "Bio-mediated soil improvement," Ecological Engineering, vol. 36, pp. 197–210 (2010).

[2] C. Geindreau et al., "Mechanical and Microstructural Changes of Biocemented Sand Subjected to an Acid Solution," International Journal of Geomechanics, vol. 22, (2022).

[3] M. Sarkis, et al., "D.E.M. modeling of biocemented sand : Influence of the cohesive contact surface area distribution and the percentage of cohesive contacts," Computers and Geotechnics, vol. 149, p. 104860, (2022).

Imaging solute transport in 3D printed porous media

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Keywords: Refractive Index Matching, Stereolithography , PLIF, Solute transport

Solute transport in porous media is a key process for many natural and industrial processes, such as contaminant transport in the subsurface, and chromatography and catalysis in reactors.

Some numerical studies [1] have shown that simple geometric parameters like bead-pack orientation with respect to the mean flow direction have a strong effect on mixing efficiency, and thus on solute transport properties. Yet, this has not been directly observed experimentally.

Imaging solute mixing inside natural opaque porous structures would require Xray imaging at high Péclet number, a configuration that is not trivial to setup. Here, we present a different approach consisting in 3D printing natural porous architectures in transparent resins and using planar laser induced fluorescent imaging (PLIF), which has shown strong benefits for quantifying solute concentration fields [2] in bead packs, but not yet in more complex porous structures.

Manufacturing of porous architectures with shapes and dimensions unreachable with classical machining processes is now available with additive manufacturing as SLA. We show that 3D printed porous materials can have transparency in a large range of the visible spectrum. We detail the methods used to optically match the fluids and the printed porous media to achieve PLIF (fig.1), and we demonstrate that this technique can be used to characterize solute transport and mixing in complex architectures.

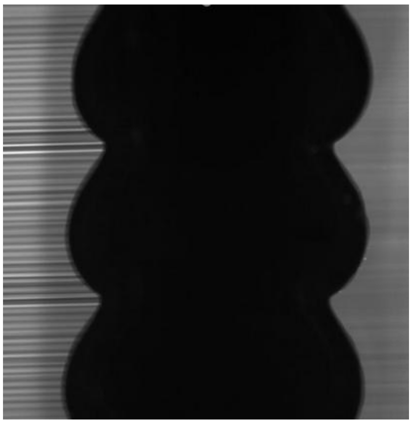

Figure 1: Fluorescence signal intensity distribution before and after propagation through a Formlabs resin curved wall

References

[1] Turuban et al. "Chaotic mixing in crystalline granular media." *Journal of Fluid Mechanics* 871, 562-594, (2019)
[2] Heyman, et al. "Stretching and folding sustain microscale chemical gradients in porous media." *Proceedings of the National Academy of Sciences* 117.24: 13359-13365, (2020).

porousMedia4Foam: A Versatile Simulator for Multiscale Reactive Transport in Subsurface Environments

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Keywords: Reactive transport, Numerical modelling, Micro-Continuum Modeling, Supercritical Fluids, Multiphase Flow, Open-source code

A common thread in modeling subsurface environments is the presence of water–often in a supercritical state–transporting dissolved species or colloids and interacting with both the porous rock matrix and other fluid phases. These systems are governed by tightly coupled physico-chemical processes spanning wide ranges of spatial and temporal scales, thermodynamic conditions (pressure, temperature), and chemical compositions.

We introduce *porousMedia4Foam*, a general-purpose simulator for reactive transport in porous media, capable of modeling both pore-scale and Darcy-scale processes via a micro-continuum approach [1]. The framework supports hybrid simulations where regions governed by Stokes flow coexist with others modeled using Darcy's law.

Built upon established open-source components, the simulator employs an operator-splitting strategy to couple:

(i) advective-diffusive transport in porous media, and

(ii) chemical reactions, including dissolution, precipitation, complexation, and phase transitions.

The mechanical component extends OpenFOAM with solvers for multiscale, multiphase transport, as well as standard Darcy-scale formulations for two-phase flow incorporating relative permeability and capillary pressure relationships. The reactive transport module integrates PhreeqcRM as the chemical engine [2] .

An in-house thermodynamic database, currently under development, extends the Helgeson-Kirkham-Flowers (HKF)[3] model to high-pressure, high-temperature, and high-salinity conditions. This is supported by a robust equation of state valid in the supercritical domain [4].

porousMedia4Foam is applicable to a wide range of geoscientific and engineering problems, including resource exploitation (e.g., geothermal energy, mineral recovery, freshwater access), environmental remediation (e.g., CO_2 sequestration, aquifer decontamination), and natural hazard assessment (e.g., volcanic and seismic risk).

References

[1] Soulaine, C. et al., porousMedia4Foam: Multi-scale open-source platform for hydro-geochemical simulations with OpenFOAM, Environmental Modelling and Software, 145 (2021)

[2] Parkhurst, D. L. , Wissmeier, L., PhreeqcRM: A reaction module for transport simulators based on the geochemical model PHREEQC, Advances in Water Resources, 83, 176-189 (2015)

[3] Helgeson, H. C. et al., Theoretical prediction of the thermodynamic behavior of aqueous electrolytes by high pressures and temperatures; IV, Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600 degrees C and 5kb. American Journal of Science, 281(10), 1249-1516 (1981)

[4] Wagner, W., Pruss, A., The IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use, Journal of Physical and Chemical Reference Data, 31(2), 387-535 (2002)

Friction modifies poroelasticity of a yeast clog

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Keywords: frictional poromechanics, bioclogging, microfluidics, yeast

Soft porous media consisting of assemblies of biological objects are common in many industrial and natural situations. They are often confined, as in the case of yeast clogs trapped in a filtration membrane, or human tumor cells in the case of e.g. bone cancer. Whereas this confinement and the possible friction induced at the boundaries of the porous media are not addressed by the well-known poromechanics theory [1], some recent experimental results tend to prove their importance [2].

For this presentation, we have studied the mechanical properties of a clog of living particles based on observations at the microscale in a model configuration: we used the baker's yeast Saccharomyces cerevisiae, with known mechanical and biological properties, to form clogs that were observed in a quasi-2D microfluidic device with well-controlled dimensions to ensure a high degree of confinement [3]. After the formation of a clog, compression and decompression cycles were applied (see Fig. 1), both in a flow-driven configuration and in an impermeable piston-driven one. The results show that the stress-displacement relationship deviates from the predictions of poromechanics theory and conventional interpretations in the literature, revealing a strong hysteresis. This is the signature of energy loss during the compression-decompression cycle. In addition, complementary experiments show that stress is stored during decompression.

A continuous model is proposed which takes into account the coupling between the fluid flow, the deformation of the clog and the friction against the device's walls. This reveals that the friction magnitude is dictated by a single dimensionless number, that is proportional to the friction coefficient multiplied by the aspect ratio of the device. This model reproduces all the observations remarkably well. Taken together, these results provide a first theoretical framework for the study of bioclogging on small scales and show that friction can have non-trivial effects on the mechanics of confined deformable porous media.

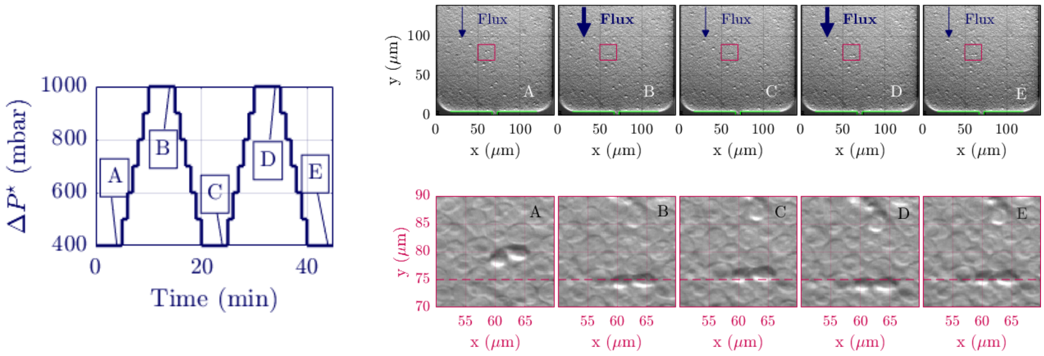

Figure 1: Left: pressure signal evolution during two cycles. Top-right: micrograph of the clog during pressure evolution at times labelled A-E. Bottom-right: zoom on the pink square of the corresponding top-right pictures.

References

[1] C.W. MacMinn, E.R Dufresne, J.S. Wettlaufer, Physical Review Applied, 2016, 5, 4.
[2] T. Lutz, PhD Dissertation, 2021, Yale Graduate School of Arts and Sciences, New Haven, USA.
[3] T. Desclaux et al., Physical Review Fluids, 2024, 9, 3, 034202.

Thermodynamic and Structural Insights into Water Intrusion in ZIF-8 Using Calorimetry and Neutron Diffraction

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Keywords: Thermodynamics, Confinement, Intrusion, energy storage

The filling of nanopores by a fluid is governed by both surface interactions and pore morphology. For hydrophobic materials, this process—known as liquid intrusion—requires the application of external pressures significantly higher than atmospheric. Various porous materials with different topologies and surface chemistries, including post-grafted mesoporous silicas, MOFs, and zeolites, are commonly studied in this context [2].

Here, we investigate the intrusion of water into the well-known metal-organic framework ZIF-8 [3] using a combination of experimental techniques. High-pressure calorimetry [1] is employed to quantify the heat exchanged during intrusion at room temperature and to probe potential phase transitions of either the confined fluid or the host matrix. In parallel, high-pressure neutron diffraction provides structural insight into the intruded liquid and its transformations.

In both approaches, we observe good agreement in the pressure–temperature location of key thermodynamic events, such as intrusion pressures and phase transitions. This combined analysis offers a new perspective on applied and fundamental questions concerning energy storage and thermodynamics of fluids under nanoconfinement.

[**Erreur ! Signet non défini.**] Karbowiak, Thomas, Christian Paulin, et Jean-Pierre Bellat. « Determination of Water Intrusion Heat in Hydrophobic Microporous Materials by High Pressure Calorimetry ». Microporous and Mesoporous Materials 134, no 1-3 (octobre 2010): 8-15. https://doi.org/10.1016/j.micromeso.2010.05.001.

[**Erreur ! Signet non défini.**] Picard, Cyril. « Accumulateurs à nanoporeux lyophobes ». Innovations technologiques, mai 2017. https://doi.org/10.51257/a-v1-re266.

[**Erreur ! Signet non défini.**] Grosu, Ya., G. Renaudin, V. Eroshenko, J.-M. Nedelec, et J.-P. E. Grolier. « Synergetic Effect of Temperature and Pressure on Energetic and Structural Characteristics of {ZIF-8 + Water} Molecular Spring ». Nanoscale 7, no 19 (2015): 8803-10. https://doi.org/10.1039/C5NR01340B.

Stochastic Modeling And Simulation of Particle Bridging in Constricted Channels

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Keywords: Pore clogging, CFD-DEM, Discrete stochastic model, Particle transport

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Clogging in porous media and microfluidic systems is governed by a complex interplay of fluid dynamics, particle interactions, and geometric confinement. In this work, we investigate how specific pore-scale factors—constriction angle, particle Reynolds number, particle concentration, particle-to-constriction size ratio, and constriction smoothness—govern the stochastic behavior of clogging in semidilute suspensions.

To explore this, we employ a coupled Computational Fluid Dynamics–Discrete Element Method (CFD-DEM) framework to simulate particle transport through constricted channels. This numerical approach captures hydrodynamic interactions and particle-particle contacts in high fidelity [1]. We propose a discrete stochastic model that quantifies clogging events in terms of the number of particles (termed "escapees") that successfully pass a constriction before a stable particle arch forms.

Our findings reveal distinct trends in clogging behavior [2]. The average number of escapees systematically decreases with increasing constriction angle and particle concentration, highlighting enhanced clogging probability under confined and more crowded conditions. Interestingly, this number remains largely invariant with respect to flow rate in the low-Reynolds-number (Stokes) regime, indicating that geometry and concentration dominate over hydrodynamic forcing in this regime. Furthermore, the number of escapees before clogging increases in discrete steps with the increase of the particle-to-constriction size ratio. We also observe that smoother constrictions delay clogging and yield less stable bridges compared to sharper geometries.

The discrete stochastic model accurately reproduces these trends, offering a predictive tool that bridges simulation and theory. These insights contribute to a mechanistic understanding of particle bridging and offer guidance for designing filtration systems, porous membranes, and microfluidic devices to control or prevent clogging under various operating conditions.

References

[1] L. Maya Fogouang et al., Particulate Transport in Porous Media at Pore-Scale. Part 1: Unresolved-Resolved Four-Way Coupling CFD-DEM, *Journal of Computational Physics*, Volume 521, (2025).

[2] L. Maya Fogouang et al., Numerical investigation and stochastic modeling of particle bridging under various flow, pore and particle properties, (Under review).

Water flow and Solute Transport in Low-Cost Porous Adsorbents: Application to Olive Mill Wastewater Filtration

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Keywords: water flow, porous media, natural low-cost adsorbents, pollutant transport

The olive oil industry generates olive mill wastewater (OMW), an effluent with high organic load, strong acidity, elevated phytotoxic phenolic compounds, and considerable chemical and biochemical oxygen demands [1]. Their untreated discharge into the environment leads to soil acidification, contamination of surface and groundwater and the destruction of aquatic ecosystems. To address this environmental challenge, this work proposes water treatment filtration, using natural and low-cost adsorbents to treat OMW and promote water reuse for irrigation. Quartz sand, sawdust, straw, pozzolan and biopolymers (such as chitosan, oyster shell, argan shell…) were used as natural adsorbent and then compared with a traditional activated carbon adsorbent. These materials were characterized through physical analyses (moisture content, volatile matter, ash content, fixed carbon, bulk density and pore size distribution). Their chemical characterisation included elemental analysis such as CHNS/O, infrared and Raman spectroscopy whereas their structural analyses were performed by SEM-EDX and XRD. The overall analyses showed that straw and sawdust, with their high volatile matter content (83–85%) and moderate fixed carbon (14%), offer a limited adsorption capacity mainly through surface interactions. In contrast, activated carbon, characterized by a high carbon content (88%) and a highly porous structure, demonstrated superior adsorption properties. SEM-EDX analyses revealed a highly porous surface, XRD confirmed an amorphous structure favorable to adsorption and BET measurements indicated a high specific surface area (1024 m²/g) with dominant microporosity. These characterizations are essential for understanding the relationship between the physico-chemical properties of the adsorbents and their ability to retain pollutants. Column laboratory tracer experiments and mathematical modelling were then performed on these natural and low-cost adsorbents to investigate and quantify water and solute transport process in these solid porous media under steady state flow conditions. For this purpose, adsorbents were introduced in successive layers and/or mixed with a sand to have a homogenous distribution of the porous media into the columns. Tracer tests were performed by injecting potassium bromide (KBr) and applying inverse modeling with HYDRUS-1D using the mobile/immobile water model (MIM) to evaluate preferential flow pathways. After these tests conducted at small laboratory columns (3.3 cm in diameter and 17 cm in height) to optimize filtration conditions and study the hydrodynamic behaviour of the porous media, a semi-pilot experimental system was designed using a filtration column measuring 110 cm in height and 20 cm in diameter, filled with successive layers, including a layer of pozzolan and layers composed of a mixture of sand and selected natural adsorbent materials. Actually, semi-pilot scale experiments are underway to monitor the reduction of pollution indicators and assess the overall performance of the treatment system.

References

[1] Achak M., Hafidi A., Ouazzani N., Sayadi S., Mandi L., Low-cost biosorbent "banana peel" for the removal of phenolic compounds from olive mill wastewater: kinetic and equilibrium studies, *Journal of Hazardous Materials*, 166, 117–125 (2009).

Fluid transfers through *dynamic NMR relaxometry*

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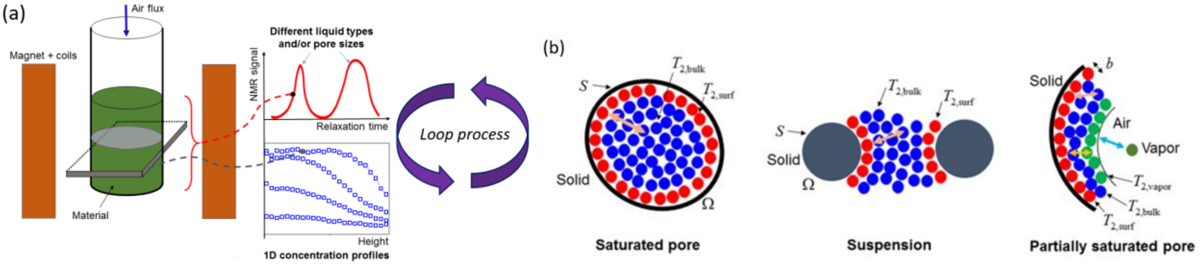
Keywords : low field NMR, relaxation time, NMR profile, hydric transfer, biobased material, smooth material

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.

Figure



References

[1] Maillet, B.; Sidi-Boulenouar, R.; Coussot, P. Dynamic NMR Relaxometry as a Simple Tool for Measuring Liquid Transfers and Characterizing Surface and Structure Evolution in Porous Media. *Langmuir* 2022, 38, 15009–15025.

[2] B. Maillet, G. Dittrich, P. Huber, P. Coussot, Diffusion-like drying of a nanoporous solid as revealed by Magnetic Resonance Imaging, *Physical Review Applied,* 18, 054027 (2022)

[3] Cocusse M, Rosales M, Maillet B, Sidi-Boulenouar R, Julien E, Caré S, Coussot P (2022). Two-step diffusion in cellular hygroscopic (plant-like) materials. Science Advances, 8:eabm7830. DOI: 10.1126/sciadv.abm7830

[4] E. Julien, B. Maillet, L. Tocquer, S. Aime, P. Coussot.Dynamic NMR relaxometry as a straightforward measurement of concentration variations in colloidal gels. Submitted

Advantages of physics neural networks for modeling seawater intrusion in coastal aquifers

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Keywords: Seawater Intrusion, Coastal Aquifers, Physics-Informed Neural Network (PINNs)

Modeling seawater intrusion in coastal aquifers is a significant challenge, particularly in areas with high population density and growing pressure on freshwater supplies. Seawater intrusion occurs when saltwater encroaches into freshwater zones, disrupting the balance and quality of water resources. Accurate modeling is essential for effective water resource management and long-term sustainability.

The increasing application of artificial intelligence in scientific research has introduced new opportunities for modeling complex environmental phenomena. Machine learning techniques can generate reliable predictions by learning from existing datasets without requiring complete knowledge of the physical processes involved. However, these models often depend on large amounts of data, which can be difficult and costly to obtain. They are also typically limited in interpretability and may not perform well when applied to new or unseen conditions.

To address these limitations, Physics-Informed Neural Networks (PINNs) incorporate physical laws directly into the training of neural networks. By including governing equations, such as partial differential equations, within the model's loss function, PINNs can produce predictions that remain consistent with known physical behavior. This approach enables accurate modeling even when data availability is limited, making it highly effective in domains like seawater intrusion.

In this study, PINNs were used to model seawater intrusion through three approaches. In the first approach, the model was trained without any data to evaluate its ability to solve the governing equations independently. In the second, a small amount of pressure head and concentration data was included to improve the accuracy of predictions. In the third, only pressure head data was provided, and the model was used to estimate both pressure head and concentration, which is not feasible using conventional models based solely on data.

References

[1] Raissi, M., Perdikaris, P., Karniadakis, G.E., 2019. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J. Comput. Phys. 378, 686–707.

[2] Lehmann, F., Fahs, M., Alhubail, A., Hoteit, H., 2023. A mixed pressure-velocity formulation to model flow in heterogeneous porous media with physics-informed neural networks. Adv. Water Resour. 181, 104564. https://doi.org/10.1016/j.advwatres.2023.104564

[3] Karniadakis, G.E., Kevrekidis, I.G., Lu, L., Perdikaris, P., Wang, S., Yang, L., 2021. Physics-informed machine learning. Nat. Rev. Phys. 3, 422–440. https://doi.org/10.1038/s42254-021-00314-5.

Fluctuations enhance diffusive transport in nanopores

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Keywords: Fluctuations, nanopores, diffusion, molecular Dynamics

Abstract: Fluctuations are ubiquitous in bio and artificial nanopores: they affect ion transport through ion channels on the cell membrane barrier, particle transport inside nano-porous media, and water transport through nanoporous membranes for filtration. Fluctuations have important consequences on transport that are subtle and intricate. Most of the time, fluctuations are seen as a negative feature that impedes for example signal measurements. Yet, biological pores such as ion channels are still able to achieve complex tasks in spite of fluctuations.

To investigate the riddle of fluctuations in confined transport, here we explore how surface fluctuations of the confining interface affect particle transport nearby or within the pore. We show theoretically that dynamic fluctuations of the interface can transfer momentum to the neighboring diffusing particles, and enhance their long time diffusion coefficient [1]. This effect is all the more important in dense suspensions [2]. Using molecular dynamics, we show that such effects persist at the molecular scale, and also enhance a particle's local mobility near the interface [3]. Remarkably, at the molecular scale, other effects such as a membrane's elasticity or fluidity, do not affect motion significantly.

These results could open new avenues in artificial designs, where fluctuations are harnessed to improve transport and sensing.

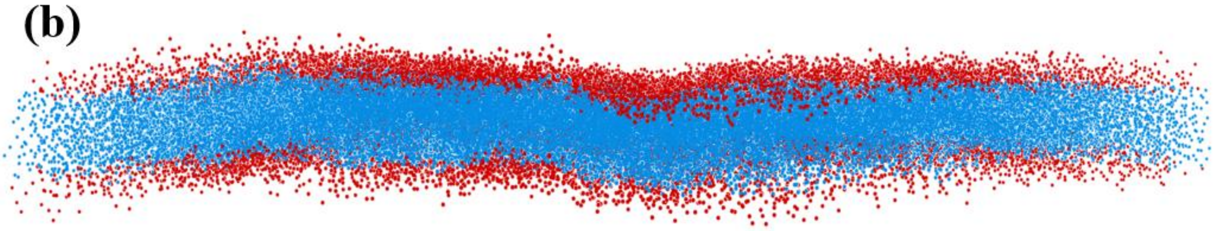

Figure: Depiction of a molecular dynamics simulation of a fluctuating membrane. Particle motion in its vicinity (not shown) is affected by membrane fluctuations. Red (blue) particles represent hydrophilic (phobic) membrane particles.

References

[1] Marbach, S., Dean, D. S., & Bocquet, L., Transport and dispersion across wiggling nanopores. *Nature Physics*, *14*(11), 1108-1113 (2018).
[2] Wang, Y., Dean, D. S., Marbach, S., & Zakine, R. Interactions enhance dispersion in fluctuating channels via emergent flows. *Journal of Fluid Mechanics*, *972*, A8. (2023).
[3] Mohammadi, A, Li Z, Marbach S. & Abbas M. Molecular motion near a soft fluctuating membrane, *to be submitted* (2025).

Machine Learning For Geochemistry And Application To Thermal Reactive Transport

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Keywords: Machine Learning, Geochemistry, Reactive Transport

Modeling reactive transport in porous media is computationally intensive, largely due to the repeated and parallel evaluation of geochemical equilibrium throughout simulations. To address this bottleneck, various machine learning strategies are being explored to replace traditional calculations with fast, predictive models. Two main approaches have emerged: intelligent adaptive tabulation methods, such as ISAT, and models based on deep neural networks. Both aim to approximate the reference geochemical equilibrium — typically solved using nonlinear solvers — with a more robust and efficient surrogate.

Our work focuses on the development and implementation of neural network-based surrogate models, trained on a large dataset generated offline using the `Arxim` geochemistry code. The training data spans a wide range of physical parameters, enabling the model to be used in large-scale simulations at the reservoir or basin scale while preserving accuracy and ensuring the stability of the reactive transport solver. The learning pipeline was developed in Python using standard libraries, and the resulting model was integrated into a custom finite volume reactive transport code also written in Python. This code couples thermal processes, fluid flow, solute transport, and geochemistry using a sequential operator splitting approach. The work was conducted by Jiusen Chen as part of his Master's internship.

While the methodology is broadly applicable, it requires careful attention to the scaling of input and output variables, selection of key features, and sampling strategies. A strong understanding of the system's physical behavior and governing equations is essential in identifying and correcting key sources of error.

We will present the methodology in detail, along with results from both offline validation (physical and statistical) and coupled reactive transport simulations on synthetic 2D test cases. Finally, we will discuss current efforts and future directions aimed at improving the approach.

References

[1] Chen, J. (2024). Méthodes d'apprentissage des modèles géochimiques et application au transport réactif. Master's internship report, Université de Paris-Cité, IFP Energies nouvelles, Rueil-Malmaison.

[2] Pope, S. B. (1997). Computationally Efficient Implementation of Combustion Chemistry Using In Situ Adaptive Tabulation. Combustion Theory and Modelling, 1(1), 41-63.

[3] Qu, J., Faney, T., Hemptinne, J.-C., Yousef, S., Gallinari, P. (2023). PTFlash: A Vectorized and Parallel Deep Learning Framework for Two-Phase Flash Calculation. Fuel, 331, 125603.

[4] Collard, N., Faney, T., Teboul, P.-A., Bachaud, P., Cacas-Stentz, M.-C., Gout, C. (2023). Machine Learning Model Predicting Hydrothermal Dolomitisation for Future Coupling of Basin Modelling and Geochemical Simulations. Chemical Geology, 637, 121676.

[5] De Lucia, M. and KÃ¼hn, M. (2021). DecTree v1.0 - chemistry speedup in reactive transport simulations: purely data-driven and physics-based surrogates. Geoscientific Model Development, 14(7), 4713-4730.

[6] Moutte, J., Michel, A., Battaia, G., et al. (2010). Arxim, a library for thermodynamic modeling of reactive heterogeneous systems, with applications to the simulation of fluid-rock systems. In: Proceedings of the 21st IUPAC International Conference on Chemical Thermodynamics.

Flow induced intermittent transport shapes colloids filtration in complex media

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Keywords: microfluidics, colloidal filtration, heterogeneity

The retention of colloids in porous media is controlled by transport through complex porous structures and deposition over its solid surfaces. Classical approaches do not capture the behaviours observed experimentally in complex media, since a key assumption is that individual attachment events happen at constant rate over defined spatial scales. Yet, due to the porous spatial variability, the role of microscopic structure on macroscopic transport and filtration remains poorly understood. Here, we develop a microfluidics model system to observe across spatial scales (from tens of microns to a meter) the transport and deposition of a mono-dispersed colloidal suspension constantly injected through a porous system of controlled heterogeneity. By tracking individual colloidal particles within the pores, we show that they move along trajectories with intermittent behaviour jumping between alternating states, each of which we call flight and dive. The first corresponds to the particle transported by the local fluid velocity through pores far enough from any solid surface not to get retained. The second corresponds to colloids traveling close enough to a grain surface so that they can interact with it and eventually attach. Due to the medium heterogeneity, the spatial extension of each state is broadly distributed. We rationalize this remarkable observation by proposing a novel stochastic model based on Continuous Time Random Walk (CTRW) that, honouring the observed intermittent behaviour and being fed only via measured parameters, bridges the microscopic medium structure and macroscopic filtration. Our model capture how microscale medium structure and complex flow are coupled with colloidal retention to control macroscopic Deposition Profiles.

Thin Film Flow: Fluid Transport via Thin Liquid Films in Slow Porous Media Flows

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Keywords: Porous media flows, Film flow, Drainage

In porous media, fluid transport typically occurs through an interconnected network of pore bodies and throats, referred to here as the *primary network*. During drainage, when a non-wetting phase displaces a wetting phase (e.g., air displacing water in a porous rock), thin films of the wetting phase often remain adhered to grain surfaces. Under certain conditions, these residual films can merge to form a *secondary network* composed of interconnected films and capillary bridges. This network can significantly enhance the medium's connectivity and create additional pathways for fluid transport, beyond those of the primary network [1-3].

We present experiments performed in transparent, micromodel-like porous networks that allow for direct visualization of these secondary pathways. Our observations show that fluid domains disconnected in the primary network can become effectively connected via thin films. This alternative transport mechanism has important implications for environmental and geophysical processes, including pollutant dispersion in soils and nutrient delivery to plant roots in dry conditions. Additionally, we will present preliminary results indicating that transport through thin films can play a significant role in mixing processes within porous media, further underlining their functional importance.

References

[1] M. Moura, E. G. Flekkøy, K. J. Måløy, G. Schäfer and R. Toussaint, Connectivity enhancement due to film flow in porous media, *Phys. Rev. Fluids* **4**, 094102 (2019).
[2] P. Reis, M. Moura, G. Linga, P. A. Rikvold, R. Toussaint, E. G. Flekkøy, K. J. Måløy, A simplified pore-scale model for slow drainage including film-flow effects*, Adv. Water Resour.* **182**, 104580 (2023).
[3] P. Reis, G. Linga, M. Moura, P. A. Rikvold, R. Toussaint, E. G. Flekkøy, and K. J. Måløy, Interaction between corner and bulk flows during drainage in granular porous media, *Adv. Water Resour.* **198**, 104914 (2025)

Eliminating Contact Angle in Pore-Scale Two-Phase Flow: An OpenFOAM-Based Approach

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Keywords: Two-phase flow, Wettability, Wetting film, Lubrication, Pore scale

Multiphase flow in porous media occurs in a variety of scenarios, including subsurface flow in contaminant-polluted aquifers, undersaturated petroleum reservoirs, and gas storage in aquifers. Wetting conditions are key to describing the displacement of menisci within the pore space and are typically characterized by the contact angle. However, variations in fluid composition, pH, and salinity can lead to non-monotonic changes in the contact angle, limiting the predictive capability of this approach. As an alternative, a lubrication model combined with disjoining pressure can be used to describe wetting behavior. This method accounts for intermolecular interactions directly, without relying on the concept of contact angles [1].

In this work, we present a new OpenFOAM-based pore-scale simulator for two-phase flow that eliminates the need for the contact angle concept. The framework combines a Volume of Fluid (VOF) solver to track the fluid–fluid interface with a lubrication model to capture thin-film dynamics at the solid boundaries. The velocity of the thin film is imposed as a boundary condition for the VOF simulations. The lubrication model is governed by a partial differential equation involving a bi-Laplacian operator, which is solved in OpenFOAM using the Moving Least Squares method. We demonstrate the capabilities of the simulator by modeling drainage and imbibition processes at the pore scale, as well as wettability alteration resulting from changes in pH and salinity.

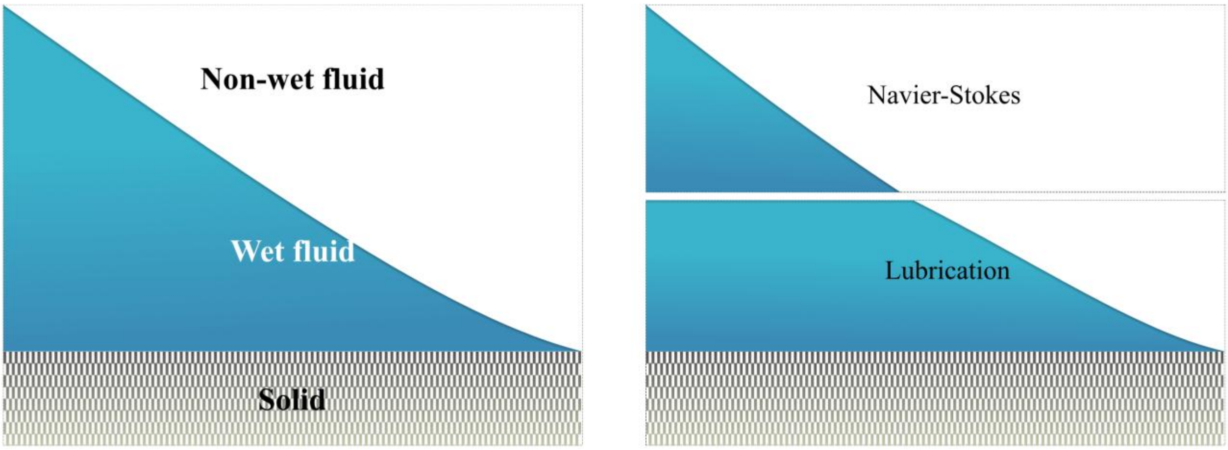

Figure 1: Schematic of contact region modeled by coupling of lubrication model and Navier-Stokes.

Reference

[1] Norouzisadeh, Mojtaba, Philippe Leroy, and Cyprien Soulaine. "A lubrication model with slope-dependent disjoining pressure for modeling wettability alteration." Computer Physics Communications 298 (2024): 109114.

Progressive clogging via dendrite growth in porous media

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Keywords: colloid, dendrite, clogging, microfluidics, porous media, permeability damage

The transport of colloidal particles in porous media governs deposition and clogging mechanisms that significantly impact flow efficiency in both natural and engineered systems. Yet, the contribution of dendritic structures—a unique deposition morphology—to clogging dynamics is still poorly explored. Understanding the formation and growth of dendrites is essential for advancing clogging dynamics and assessing their impact on permeability. Using microfluidic flow experiments coupled with computational fluid dynamics, we investigate this dendrite-based clogging mechanism in a heterogeneous, tortuous porous domain. Our results reveal a novel clogging mechanism—dendrite clogging—where a single deposition site initiates a structure that extends across the pore space, bridging grains and causing complete clogging (Figure 1). Unlike previously described aggregation-based clogging, which involves multiple deposition sites, dendrite clogging evolves from a single-site deposition. Through hydrodynamic and adhesive torque balance analysis, we develop a flow-dependent criterion that predicts dendrite formation. Our results demonstrate that moderate flow rates favor multilayer deposition in front-cone stagnation zones, triggering dendrite growth and abrupt permeability loss. In contrast, higher flow rates suppress dendrite formation, resulting in more gradual permeability decline, well described by the Verma–Pruess permeability-porosity model. These insights establish a predictive framework for dendritic deposition under different flow conditions. They also shed light on previously unexplored clogging mechanisms, contributing to a deeper understanding of clogging in porous media with implications on optimizing flow in systems such as filtration, groundwater transport, and biomedical microfluidics.

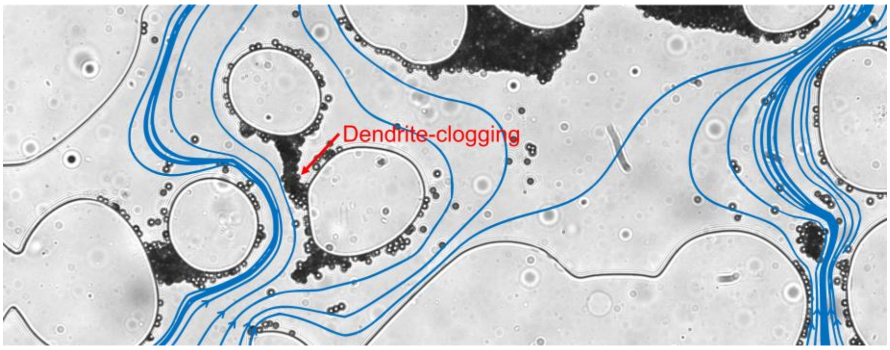

Figure 1: Formation of a dendrite-clogging structure bridging grains in a porous medium, with blue streamlines illustrating flow redirection.

Modeling Approaches For Drainage Instabilities In Porous Media: Phase-Field Versus Dynamic Capillary Pressure Model

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Keywords: drainage, fingering instabilities, dynamic capillarity, phase field modeling

The invasion of a non-wetting fluid into a porous medium initially saturated with a wetting fluid is a common phenomenon in multiphase porous media flow, often resulting in a moving interface known as a drainage front. Such fronts appear in transient processes like supercritical CO_2 injection into brine-saturated formations or intense drying of water-saturated clays. Under favorable conditions such drainage front is known to destabilize resulting in finger-like instabilities [1] with specific morphological properties and scales depending on the regime of the flow. Broadly the stability of a drainage front is hypothesized [1, 2, 3, 4] to be governed by a balance between capillary, viscous, and gravitational forces.

In this work, we focus on the capillary effect and in a practically relevant regime where the invading fluid is significantly less viscous and dense than the defending fluid. Moreover we restrict ourselves to macroscopic continuum-scale modeling of the phenomenon. Classical poromechanical framework describes the capillary pressure difference between the immiscible pore fluids as a local bijective function of the saturation degree of the wetting fluid, $P_c(S_w)$. Two corrections were proposed in the literature ([5] and [6]), that intend to enrich the otherwise rough up-scaling of the capillary retention relation in the classical model. These models seem to successfully describe macroscopic flow instabilities, nevertheless in the imbibition case ([7] and [8]) and with the drastic simplifying hypothesis of neglecting non-wetting phase pressure that is relevant to certain applications such as soil hydrology. The models' relevance and comparative performance when it comes to drainage have note yet been investigated.

In this work we first reintroduce the non-wetting phase pressure as an independent variable and present the dimensionless structure of both the models. Then we show numerically and in 1D the emergence of self-similar traveling wave solutions during drainage under certain regimes for both these models. Further we conduct linear stability analyses of these solutions against transverse perturbations to study their susceptibility to asymptotic growth of those perturbations and thus revealing conditions under which these enriched models capture physically consistent fingering instabilities. Thus this study brings stability analysis one step closer to practically relevant scenario of compressible drainage flow.

References

[1] Lovoll, G., Méheust, Y., Maloy, K.J., Aker, E., & Schmittbuhl, J. (2005). Competition of gravity, capillary and viscous forces during drainage in a two-dimensional porous medium, a pore scale study. Energy, 30, 861-872.

[2] Saffman, P.G., & Taylor, G.I. (1958). The penetration of a fluid into a porous medium or Hele-Shaw cell containing a more viscous liquid. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 245, 312 - 329.

[3] Homsy, G. (1987). Viscous fingering in porous media. Annual Review of Fluid Mechanics, 19, 271-311.

[4] Wang, Z., Feyen, J., & Elrick, D.E. (1998). Prediction of fingering in porous media. Water Resources Research, 34, 2183 - 2190.

[5] Hassanizadeh, S.M., & Gray, W.G. (1990). Mechanics and thermodynamics of multiphase flow in porous media including interphase boundaries. Advances in Water Resources, 13, 169-186.

[6] Sciarra, G. (2016). Phase field modeling of partially saturated deformable porous media. Journal of The Mechanics and Physics of Solids, 94, 230-256.

[7] Eliassi, M., & Glass, R.J. (2003). On the porous continuum-scale modeling of gravity-driven fingers in unsaturated materials: Numerical solution of a hypodiffusive governing equation that incorporates a hold-back-pile-up effect. Water Resources Research, 39.

[8] Ommi, S.H., Sciarra, G., & Kotronis, P. (2022). A phase field model for partially saturated geomaterials describing fluid-fluid displacements, Part II: Stability analysis and two-dimensional simulations. Advances in Water Resources.

Reactive Percolation In Ultramafic Rocks: Impacts Of Permeability And Pore Structure On Hydrogen Generation

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Keywords: Reactive Transport, Microtomography, Serpentinization

Hydrogen production is attracting growing interest in response to current environmental and economic challenges. Among the approaches being explored, stimulated hydrogen production (orange hydrogen, Fig. 1) relies on serpentinization reactions triggered by the injection of an aqueous solution into a massif of ultramafic mantle rocks (i.e., peridotites). The hydration and oxidation reactions taking place during serpentinization lead to the transformation of ferrous iron (Fe^{2+}) to ferric iron (Fe^{3+}) and is accompanied by the generation of H_2 (Fig. 1).

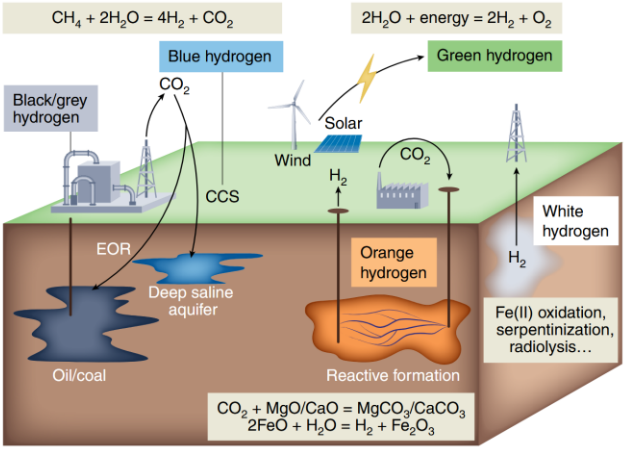

Figure 1: The different colours of hydrogen [1].

H_2 generation during serpentinization has been extensively studied through batch experiments conducted on isolated minerals or rock powders. These materials strongly simplify the petrophysical complexity of a natural peridotite, which generally exhibits a low permeability and heterogeneous pore network geometry. During the alteration, the variable reaction kinetics controlled by local fluid flow and mineral properties (texture, composition) lead to petrophysical changes that can, in turn, impact the extent of the alteration. To overcome these limitations, an experimental setup was developed on the MIMAROC platform using a reactive percolation cell in which water circulates through the rock sample at temperatures ranging from 100 to 150°C. This setup enables real-time 3D X-ray microtomography and fluid geochemical characterization, and allows linking the evolution of permeability to the structural transformations in the pore network, depending on the degree of reaction and associated serpentine precipitation.

These results improve the understanding of mineralogical and petrophysical changes driven by serpentinization, supporting the development of large-scale orange hydrogen production [1].

References

[1] Osselin, F., Soulaine, C., Fauguerolles, C., Gaucher, E. C., Scaillet, B., Pichavant, M., Orange hydrogen is the new green. Nature Geoscience 15, 765–769 (2022).

Evaporation Of A Sodium Chloride Aqueous Solution From A Porous Medium: Dome Efflorescence Formation

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Keywords: salt crystallisation, porous medium, evaporation

The study of the crystallization of one or more salts resulting from evaporation from a porous medium has motivated numerous works, see [1] and references therein. However, a systematic study of the impact of the evaporation conditions and the mean pore size of the porous medium is still lacking. In order to fill this gap, we are performing an experimental campaign for aqueous solutions of sodium chloride where both factors are varied. As illustrated in Fig.1, the considered evaporation process typically leads to the formation of a salt structure developing at the evaporative surface of the porous sample. This type of salt structure is referred to as a salt efflorescence [1, 2]. The developed experimental set-up allows us to determine the drying kinetics, to characterize the growth of the efflorescence and to get insights into the internal structure of the efflorescence via X-ray microtomography (Fig.1). The drying kinetics is typically characterized by two main stages. In the first stage, the evaporation rate is comparable to the one for pure water. In the second stage, the evaporation rate becomes much lower. These two stages can be correlated to the efflorescence growth with also exhibits two main stages with a first stage of fast growth compared to the second stage of much slower growth. As illustrated in Fig.1, a remarkable feature in these experiments is that the efflorescence is not only itself a porous medium but also a hollow structure, referred to as a dome structure. The features, i.e., the drying kinetics, the efflorescence growth and the dome formation will be discussed in relation with the various experiments performed and recent results in the literature discussing the efflorescence detachment process [3].

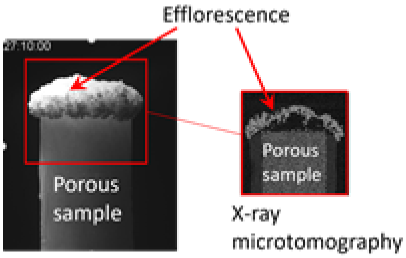

Figure 1: Exemplary efflorescence dome forming in the performed evaporation experiments

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References

[1] Salt Crystallization in Porous Media, coordinated by H.Derluyn and M.Prat, ISTE-Wiley (2024)
[2] H. Eloukabi, N.Sghaier, S. Ben Nasrallah, M.Prat, Experimental study of the effect of sodium chloride on drying of porous media: the crusty-patchy efflorescence transition. Int. J. of Heat and Mass Tr. 56, 80–93 (2013).
[3] G Licsandru et al. Detachment mechanism and reduced evaporation of an evaporative NaCl salt crust. Scientific Reports 12 (1), 7473 (2022).

3D Vizualization Of Fast Two-Phase Flows In Porous Media Using A Laboratory X-Ray CT Scanner

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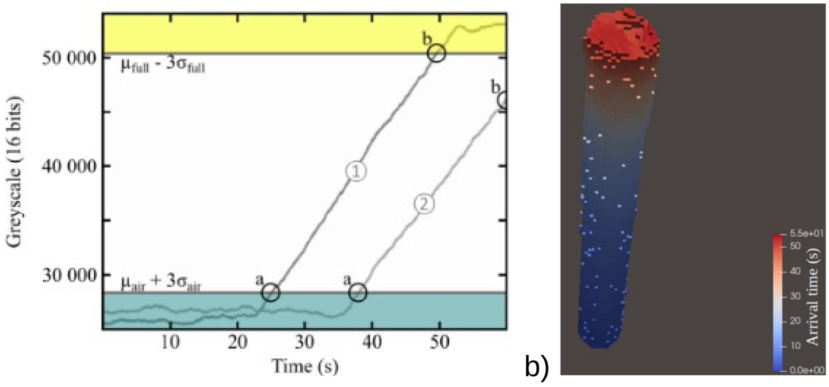
Keywords: Imbibition, X-Ray CT, Image analysis, porous media

This study aims at exploring the capability of a standard laboratory X-Ray CT scanner to provide detailed 3D observation of a fast two phase flows. Considering the case of a liquid invading a dry capillary tube or porous media, the flow is considered fast if the liquid front propagates in the whole field of view with a characteristic time of the same order of magnitude or faster than the acquisition time required to compute a reliable X-Ray tomography. This configuration is generally considered inappropriate for classical X-Ray CT imaging: Any area of the sample that undergoes a change in the nature of the fluid during acquisition will appear blurred in the reconstructed image. The proposed methodology aims at taking advantage of this effect by (I) continuously acquiring X-ray radiographies, (ii) applying the reconstruction algorithm to successive sets of radiographies similarly to sliding averages, (iii) performing an analysis of the CT value signal dynamics in each voxel (Fig. 1.a). This method allows to estimate accurately the arrival time of the liquid in each voxel (Fig. 1.b).

To illustrate the capability of the method, the CT scanner held in the 3SR lab was pushed to its limits with a tomography acquired in about 30s with 600 projections of 384x480 pixels (using a 4x4 binning mode). The 3D field of view was about 1.2x1.2x1.5 cm with a voxel size of 35 μm. A typical experiment lasted 60s. The analysis required the computation of about 1200 tomographies. Different test cases were considered using 3D printed samples including one or several capillary tubes and a model porous media. Water and Ucon oil were used to explore a wide range of viscosity and surface tension. Imposed flow and free capillary rise were considered. Even if the method requires an optimization of experimental parameters and computational cost, it offers very promising perspectives to extend the capabilities of laboratory CT scanner to study dynamic processes in porous media.



a) b)

Figure 1: Free capillary rise in a pipe (a) Example of CT signal dynamics in 2 voxels, (b) Arrival time 3D map inside the pipe obtained after image processing.

Acknowledgement: *This project was supported by UGA programs CDP Musitox and Labex Tech21.*

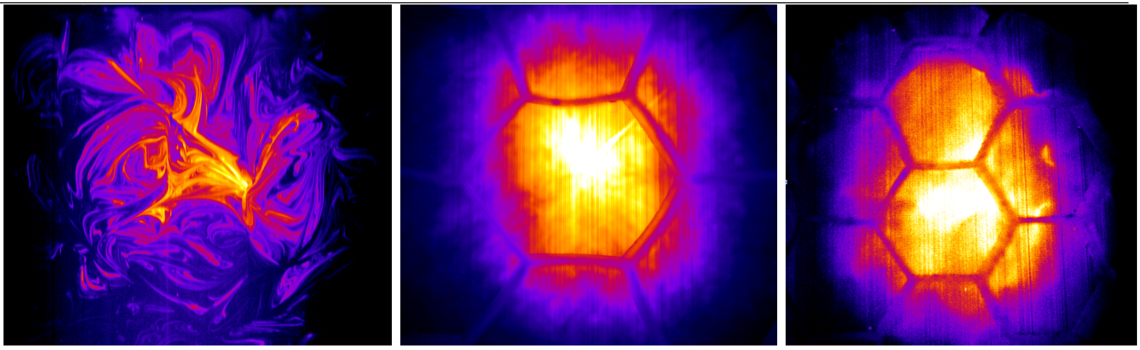


Figure 1: Transverse cross-section of conservative tracer concentrations (color scale) imaged via the push-pull technique [2]. (left) at pore scale (from [2]) (middle) at Darcy scale in homogeneous sand (right) at Darcy scale in the presence of inclusions.

Imaging Of Solute Transport Through Impermeable Inclusions At Darcy Scale.

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Keywords: Mixing, Transport, Heterogeneous, Chaos, Discontinuous, Darcy.

Mixing governs the fate of transported solutes across a broad spectrum of natural and engineered porous materials. The structure and geometry of the pores and the heterogeneity of the permeability field induce anomalous transport and mixing dynamics at multiple scales. At the pore scale, recent studies have shown that mixing can be controlled by chaotic advection at large Péclet numbers [2]. Such extreme conditions are not common in natural subsurface flows. Nevertheless, mixing at larger scale, such as at the Darcy scale, occurs at much larger Péclet numbers and may be strongly affected by the stirring action of a heterogeneous flow. Although Lester & al. [1] have demonstrated that no significant transverse mixing can exist in steady 3D Darcy flow with a smooth isotropic permeability field, anisotropic or discontinuous permeability fields have the potential to increase transverse mixing and generate chaotic advection. However, only a few experimental studies have reported such enhancement yet.

Here, we present an experiment to quantify the solute mixing in Darcy flows through impermeable inclusions. We image with a laser sheet the echo of a fluorescence dye, sequentially pushed and pulled by a steady flow inside an opaque porous media, a technique proposed by [2]. The porous media is formed either by homogeneous sand or by a matrix of impermeable inclusions (beads of diameters of 1 cm) surrounded by fine sand (0.1 mm). We follow the spatiotemporal distribution of concentration and the decay of scalar variance decay with advection time (Fig. 1). We find that the presence of inclusions enhances the transverse mixing of the tracer and that the scaling laws do not obey the classical dispersive transport laws. Our preliminary experimental results shed new light on the mechanisms of mixing at large scales.

References

[1] Lester & al, Under What Conditions Does Transverse Macrodispersion Exist in Groundwater Flow?, Water Resources Research, 59 (2023)

[2] Heyman, J., Lester, D. R., & Le Borgne, T. (2021). Scalar signatures of chaotic mixing in porous media. Physical Review Letters, 126(3), 034505.

^{19}F Magnetic Resonance Imaging-Informed Modelling of PFAS in Porous Media

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Keywords: PFAS, MRI, transport, porous media

Per- and polyfluoroalkyl substances (PFAS) are persistent contaminants. Predicting their fate in natural porous media such as soils is critical to developing effective contaminant management strategies. To this day, knowledge regarding transport processes of PFAS in porous media mostly relies on the measurement of breakthrough curves (BTCs), i.e. time evolution of the outflow concentration of the contaminant under scrutiny [1]. However, the inference of transport mechanisms from a BTC may not be unique, since this curve results from all the processes occurring within the porous media.

We addressed this issue using ^{19}F magnetic resonance imaging (MRI), with a simple approach to remove J-coupling between non-equivalent ^{19}F atoms that hinders accurate measurements [2], to monitor the transport of perfluorobutanoic acid (PFBA) within a sand-packed column. A transport model including PFBA sorption reproduced well the BTC, while the time- and space-resolved ^{19}F MRI data were better fitted without considering any sorption. We were able to show that this discrepancy is due to an imperfect column exit that was responsible for a slight asymmetry of the BTC [3]. Despite the small uncertainties affecting the ^{19}F MRI signal, we were able to confidently distinguish between the two transport models. This work highlights the benefit of combining MRI with transport modelling and it paves the way for the handling of even more complex experimental situations.

References

[1] Sardin, M., Schweich, D., Leij, F. J., & Van Genuchten, M. T., Modeling the nonequilibrium transport of linearly interacting solutes in porous media: A review, *Water Resources Research*, 27(9), 2287-2307 (1991).
[2] Aguilar, J. A., Nilsson, M., Bodenhausen, G., & Morris, G. A., Spin echo NMR spectra without J modulation, *Chemical Communications*, 48(6), 811-813 (2012).
[3] Raimbault, J., Peyneau, P. E., Courtier-Murias, D., Bigot, T., Gil Roca, J., Béchet, B., & Lassabatère, L., Investigating the impact of exit effects on solute transport in macroporous media, *Hydrology and Earth System Sciences*, 25(2), 671-683 (2021).

Coupled Thermo-Hydro-Mechanical uncertainties for CO_2 storage integrity assessment

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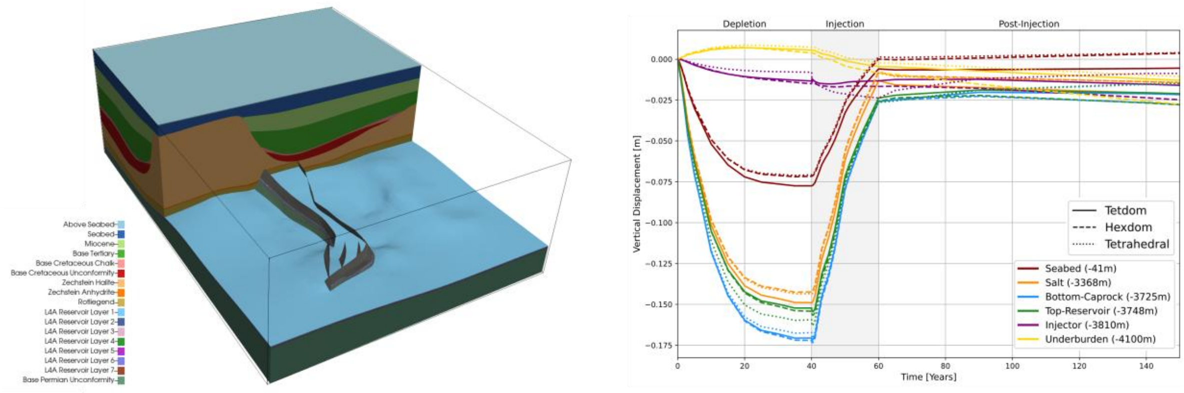
Keywords: THM, Geomechanics, CO_2 Storage, Uncertainty analysis, Meshing strategies

The Aramis project in the Netherlands is a key initiative in CCS, where industrial actors aim to reduce CO_2 emissions by capturing and storing it in a depleted offshore gas field under the North Sea. This study focuses on geomechanical risk assessment in a realistic setting, considering both the depletion and injection phases. The geological domain includes a depleted reservoir bound by fault surfaces and a prominent salt body, which adds complexity due to stress reorientation around its structure, as shown in Figure 1 (a).

The problem is modeled using a non-isothermal, compositional two-phase flow model, fully coupled to a linear thermo-poro-elastic formulation. This coupling ensures that variations in pore pressure and temperature directly influence the mechanical behavior of the rock and vice versa. A scenario representing a realistic quasi-operational framework is considered, with 40 years of hydrocarbon depletion followed by 20 years of CO_2 injection and 180 years of post-injection monitoring [1]. The simulations were performed using GEOS, an open-source platform designed for multi-physics modeling of coupled flow and geomechanics [2].

This study aims at exploring the effect of parameter variability on the uncertainty ranges affecting the prediction of the maximum admissible pressure, but also to assess the impact of different meshing strategies on the results, as illustrated in Figure 1 (b) with the vertical displacements evolution over time for different geometries.



(a) (b)

Figure 1: (a) Structural lithology of the field and (b) vertical displacement evolution over time for different geometries.

References

[1] Shotton, P. Aramis CO_2 storage Case Study – A Geomechanical Assessment of Containment. *Proceedings of the 16th Greenhouse Gas Control Technologies Conference (GHGT-16), (2022).*

[2] Settgast, R. et al., GEOS: A performance portable multi-physics simulation framework for subsurface applications. The Journal of Open Source Software, 9(102), 6973, (2024).

Enhancements in Large-Scale Hydraulic Flow Modeling

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ABSTRACT

In the context of climate change, accurately modeling water table dynamics is essential for studying various climate scenarios and assessing the impact of anthropogenic developments. This project, carried out in collaboration with IFPEN, I2M (University of Bordeaux), and Inria, aims to develop a modeling framework suited to watershed-scale simulations over multi-year periods.

Although Richards' equation offers a detailed and reliable description of subsurface flow, solving it at such scales is computationally infeasible. The Dupuit-Forchheimer model, by contrast, provides a simplified yet practical alternative that is computationally lightweight. Our goal is to enhance the Dupuit-Forchheimer framework to make it applicable in more realistic and complex scenarios.

In this talk, we briefly present several contributions already achieved in this project:

Pumping in a partially confined aquifer: To avoid the non-physical formation of vacuum pockets during pumping, it is necessary to account for air entrapment in the aquifer. We propose a polytropic gas model that captures the formation, merging, and splitting of air pockets [1].

Surface/Subsurface Exchange: In vertically integrated models such as the Dupuit-Forchheimer and shallow water equations, exchange processes are no longer imposed as boundary conditions but instead appear as coupling source terms. Assuming instantaneous infiltration through the vadose zone, we develop a unified model that rigorously satisfies conservation of mass and energy [2].

Hydrodynamic Dupuit-Forchheimer Regime: The classical Dupuit-Forchheimer model fails to accurately capture the discharge behavior under steep hydraulic gradients—for instance, during pumping or injection operations, or over sloped impermeable layers. By incorporating hydrodynamic pressure and following techniques used in classical shallow water wave model derivations, we propose an improved formulation that better represents the discharge decay rate [3].

This research has been supported by the GeoFun project ANR-19-CE46-0010.

Keywords: Confined aquifer; Unconfined aquifer; Congested flow; Groundwater/surface water exchanges; Non-hydrostatic flow;

References

[1] M. Parisot, Congested shallow water model: Trapped air pockets modeling, SIAM Journal on Scientific Computing 45 (6) (2023) B828–B852.

[2] M. Carreau, M. Parisot, A unified shallow water/dupuit-forchheimer model for surface and groundwater flow at drainage basin scale, working paper or preprint. `https://hal.science/hal-04918607`.

[3] M. Parisot, Derivation of weakly hydrodynamic models in the dupuit–forchheimer regime, Advances in Water Resources 199 (2025) 104933.

Capturing Multi-Scale Fracture Effects in CO2 Storage Modelling under Uncertainty

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Keywords: Uncertainty Quantification, Multi-Scale, Fractured media

Efficient CO_2 storage in the subsurface is contingent upon accurate predictions of potential leakage, particularly from fault-damaged zones, which are characterised by a complex interplay of multi-scale features [1]. Investigating these multi-scale effects is essential, as fault zone conductivity remains highly sensitive to geometrical characteristics such as fracture network connectivity, aperture distributions, and localised features like surface roughness.

A major challenge, however, lies in the presence of structural uncertainties across scales, which limit the accurate representation of fine-scale features. As a result, these are often overlooked in large-scale simulations, leading to significant modelling uncertainties in leakage predictions. This issue is compounded in sensitivity analyses, where the reliance on predefined property distributions offers limited predictive robustness when exploring geological variability. The validity of empirical models, such as the Cubic Law, is particularly uncertain when applied to upscale fracture conductivities at the fracture network and fault zone scales. Discrepancies between mechanical and effective hydraulic apertures induced by fracture roughness highlight the limitations of such models [2]. Quantifying and addressing uncertainties arising from model misspecification is critical for informed decision-making in leakage risk assessment [3].

To tackle these challenges, a new methodology is introduced for propagating uncertainty in hydraulic conductivity across scales, combining AI-driven physics corrections with data-driven approaches [4]. This builds on the uncertainty quantification framework developed in [5], which adaptively adjusts to varying levels of uncertainty in both the data and models. We demonstrate that mechanical aperture measurements alone are insufficient to capture the complexity of flow through rough fractures, and even more so in interconnected networks. To overcome this limitation, an automated geometrical correction is proposed to infer latent hydraulic aperture fields, thereby incorporating the influence of small-scale roughness and structural uncertainty into the model. The resulting local maps of hydraulic aperture and permeability, with quantified uncertainties, can then be integrated into an upscaling framework by leveraging pattern recognition and purely data-driven machine learning techniques to address larger scale and more complex fracture networks. Ultimately, this approach will enable more reliable calibration of property distributions in large-scale sensitivity analyses of fault-leakage rates, ensuring meaningful integration of small-scale uncertainties.

References

[1] R. E. Rizzo, N. F. Inskip, H. Fazeli, P. Betlem, K. Bisdom, N. Kampman, et al., Modelling geological CO2 leakage: Integrating fracture permeability and fault zone outcrop analysis, International Journal of Greenhouse Gas Control, 133:104105 (2024) https://doi.org/10.1016/j.ijggc.2024.104105

[2] T. Phillips, T. Bultreys, K. Bisdom, N. Kampman, S. Van Offenwert, A. Mascini, et al., A systematic investigation into the control of roughness on the flow properties of 3D-printed fractures, Water Resources Research, 57:e2020WR028671 (2021) https://doi.org/10.1029/2020WR028671

[3] J. Fang, B. Gong, and J. Caers, Data-driven model falsification and uncertainty quantification for fractured reservoirs, Engineering, 18:116-128 (2022) https://doi.org/10.1016/j.eng.2022.04.015

[4] S. Perez, F. Doster, J. Maes, H. Menke, A. ElSheikh, and A. Busch, When Cubic Law and Darcy Fail: Correcting Model Misspecification in Fracture Conductivities, ArXiv Preprint (2025) https://doi.org/10.48550/arXiv.2503.20788

[5] S. Perez, S. Maddu, I.F. Sbalzarini, and P. Poncet, Adaptive weighting of Bayesian Physics-Informed Neural Networks for multitask and multiscale forward and inverse problems, Journal of Computational Physics, 491, 112342 (2023) https://doi.org/10.1016/j.jcp.2023.112342

Selection of convection cells during convective instabilities in heterogeneous porous media: State of the art benchmarking

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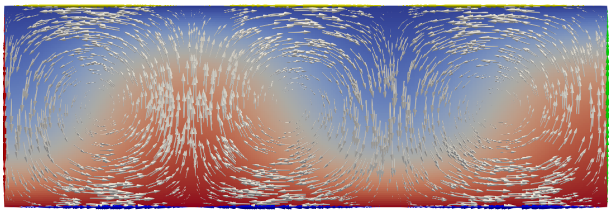
Keywords: heterogeneous porous media, thermal instability, free convection, geothermal energy

The recognition of free convection as a common and key process in geological formations over the past decades has revitalized interest in deep geothermal energy, particularly for heat extraction and solute recovery. Indeed, the convection cells localize the thermal anomaly, drive the heat and solutes transport, and control the characteristic time of thermal recharge. This process is a thermo-hydrodynamic instability known as Rayleigh-Bénard in pure fluids and Horton-Rogers-Lapwood in porous media [1, 2]. Its existence is characterized by the Rayleigh number Ra. For instability to occur, Ra must exceed a threshold that has been extensively investigated and quantified, along with the resulting heat flux [3, 8, 9]. These studies have explored various factors, including the influence of porous medium dip [5], finite-size effects [4], transport coefficients anisotropy [10, 11], boundary conditions accounting for heat and mass transfer between fault and bedrock [7]. The assumption of a Boussinesq fluid has also been partly relaxed by considering temperature-dependent transport coefficients [6, 12].

Past quantitative works most often considered homogeneous porous media. These approaches say little about the selection of unstable modes that will develop in the form of convection cells in heterogeneous media, likely to considerably increase local heat flux and solute transport in the medium. It is now quite doable to simulate free convection on large scale complex fault plane geometries. In the lack of a neat quantitative understanding, however, this approach remains extremely computationally demanding and poorly predictive [13], due to the thermoconvective instability which exponentially amplifies any perturbation, of physical and numerical nature. Here, we study the coupling between the porous medium heterogeneity (permeability, thermal diffusivity) and the hydrodynamic instability combining theoretical and numerical analysis. We characterize the large-scale effective transport coefficients, as well as the significant flow localization effects induced by the instability, which are likely to play a crucial role in facilitating geochemical transformations.

After reviewing the state of the art on onset conditions and heat flux dynamics in terms of Rayleigh and Nusselt numbers, we set up and validate a numerical model implemented in OpenFOAM [14, 15, 16]. The governing equations consist of a set of coupled Darcy-scale partial differential equations for the momentum and heat transport. The system is solved using a PISO algorithm. An example of the steady-state instability structure obtained by this simulation method is shown in the figure. The numerical constraints required to reliably resolve the onset and evolution of the instability are systematically identified. Following the approach of linear stability analysis, we examine the perturbation modes of equilibrium solutions and their impact on the onset, structure, and evolution of the instability. Toy model configurations highlight the key differences in the instability features.



Steady-state convection rolls pattern (temperature and velocity fields) simulated in a 2D 1:3 aspect ratio porous medium.

Next, we will consider heterogeneous transport coefficients to explore the localization, onset, and dynamic behavior of the instability. As a first step, we will investigate an appropriate formulation of the upscaled Rayleigh number for assessing the stability of variable-density flow in realistic, heterogeneous geologic systems — an open challenge that remains unresolved.

References

[1] C. Horton, F. Rogers, Convection currents in a porous medium, Journal of Applied Physics, 16(6), 367-370 (1945)

[2] E. Lapwood, Convection of a fluid in a porous medium, Mathematical Proceedings of the Cambridge Philosophical Society, 44(4), 508-521 (1948)

[3] W. Malkus, G. Veronis, Finite amplitude cellular convection, Journal of Fluid Mechanics, 4(3), 225-260 (1958)

[4] J. Beck, Convection in a box of porous material saturated with fluid, Physics of Fluids, 15(8), 1377-1383 (1972)

[5] S. Bories, M. Combarnous, Natural convection in a sloping porous layer, Journal of Fluid Mechanics, 57(1), 63-79 (1973)

[6] A. Zebib, D. Kassoy, Onset of natural convection in a box of water-saturated porous media with large temperature variation, Physics of Fluids, 20(4), 4-9 (1977)

[7] D. Nield, Onset of thermohaline convection in a porous medium, Water Resources Research, 4(3), 553-560 (1968)

[8] K. Aziz, M. Combarnous, Transfert de chaleur par convection dans une couche poreuse horizontale, Comptes rendus hebdomadaires des séances de l'Académie des sciences, Série B, Sciences physiques, Tome 271, 813-815 (1970)

[9] E. Palm, J. Weber, O. Kvernvold, On steady convection in a porous medium, Journal of Fluid Mechanics, 54(1), 153-161 (1972)

[10] G. Castinel, M. Combarnous, Critère d'apparition de la convection naturelle dans une couche poreuse anisotrope horizontale, Comptes rendus hebdomadaires des séances de l'Académie des sciences, Série B, Sciences physiques, Tome 278, 701-704 (1974)

[11] T. Nilsen, L. Storesletten, An analytical study on natural convection in isotropic and anisotropic porous channels, ASME Journal of Heat and Mass Transfer, 112(2), 396-401 (1990)

[12] V. Malkovsky, F. Magri, Thermal convection of temperature-dependent viscous fluids within three-dimensional faulted geothermal systems: estimation from linear and numerical analyses, Water Resources Research, 52(4), 2855-2867 (2016)

[13] F. Magri, M. Cacace, T. Fischer, O. Kolditz, W. Wang, N. Watanabe, Thermal convection of viscous fluids in a faulted system: 3D benchmark for numerical codes, Energy Procedia, 125, 310-317 (2017)

[14] H. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, Computers in Physics, 12(6), 620-631 (1998) ; OpenFOAM is an open-source computational fluid dynamics software, see https://openfoam.org

[15] P. Horgue, C. Soulaine, J. Franc, R. Guibert, G. Debenest, An open-source toolbox for multiphase flow in porous media, Computer Physics Communications, 187, 217-226 (2015)

[16] C. Soulaine, S. Pavuluri, F. Claret, C. Tournassat, porousMedia4Foam: multi-scale open-source platform for hydro-geochemical simulations with OpenFOAM, Environmental Modelling & Software, 145, 105199 (2021)

Hydro-Mechano-Chemical Coupling for the Simulation of Pore-Scale Integrity in Crystallization Process

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Keywords: Digital Rock Physics; Mineral trapping; Crystallization; Von Mises criterion; Pore-scale modeling; semi-Lagrangian methods

Carbon capture and storage (CCS) in geological formations is a promising approach to mitigating CO_2 emissions, with mineralization providing a stable, long-term solution. In this process, CO_2 dissolves in brine and reacts with minerals in the rock matrix, leading to the precipitation of stable carbonate phases. However, understanding the evolution of crystallization within the rock matrix is crucial, as it affects porosity, permeability, and mechanical integrity. Accurately modeling this process requires a detailed representation of fluid-mineral interactions at the pore scale while capturing the large-scale effects on storage efficiency and rock stability.

To address this challenge, we developed a high-fidelity numerical model using semi-Lagrangian methods [2,3] to simulate crystal growth within the porous matrix [1]. The methodology has been developed and validated for dissolution process in previsous work [5,4]. The semi-Lagrangian approach effectively handles advective transport in complex flow fields while tracking the evolution of mineral precipitation. This method allows us to resolve moving phase boundaries and capture intricate interactions between fluid flow, reactive transport, and crystal nucleation. By leveraging direct numerical simulations (DNS), we can obtain detailed insights into the dynamic evolution of mineral structures within geological formations, offering a predictive tool for assessing long-term storage performance.

Building on this framework, we have now coupled our model with the linear elasticity of the rock matrix to evaluate the mechanical stability of the storage reservoir. We compute the Von Mises stress criterion to assess whether crystallization-induced stresses exceed the rock's failure threshold, which is critical for maintaining the integrity of the formation. This approach enables us to predict potential fracturing or mechanical weakening caused by mineral growth and ensures that the CCS process remains safe and effective. By integrating fluid-mineral interactions with rock mechanics, our model provides a comprehensive tool for optimizing CO_2 mineral storage strategies in deep geological formations.

References

[1] Perez S., Etancelin J.-M., Poncet P., A semi-Lagrangian method for the direct numerical simulation of crystallization and precipitation at the pore scale, *Frontiers in Earth Science*, 13, 1493305 (2025).

[2] Perez S., Moonen P., Poncet P., On the Deviation of Computed Permeability Induced by Unresolved Morphological Features of the Pore Space, *Transport in Porous Media*, 141, 151-184 (2022).

[3] Hume L., Poncet P., A velocity-vorticity method for highly viscous 3D flows with application to digital rock physics, *Journal of Computational Physics*, 425, 109910 (2021).

[4] Molins S., Soulaine C., Prasianakis N. I., Abbasi A., Poncet P., et al., Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: review of approaches and benchmark problem set, *Computational Geosciences*, 25, 1285-1318 (2021).

[5] Etancelin J.-M., Moonen P., Poncet P., Improvement of remeshed Lagrangian methods for the simulation of dissolution processes at pore-scale, Advances in Water Resources, 146, 103780 (2020).

Optical Thermometry for Dynamic Imaging of Heat Transport in Analog Porous Media

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Keywords: heat transport, optical thermometry, porous media, local thermal non-equilibrium (LTNE)

The role of flow heterogeneity in controlling heat transfer in the subsurface remains a central question in geoscience and relevant industrial applications. Understanding it requires capturing the interplay between advection, conduction, and structural complexity of the media. In this study, we address this challenge through laboratory experiments designed to resolve pore-scale thermal dynamics relevant to applications such as geothermal energy production, aquifer thermal energy storage, and hydrology. Conventional laboratory techniques, such as thermocouples, are limited to discrete spatial sampling. Infrared imaging may offer spatial data, but strong absorption by water in the infrared range limits its ability to reliably measure fluid temperature within the flow cell. In order to resolve temperature dynamics both spatially and temporally at the pore scale, this work presents a novel application of optical thermometry as a spatially distributed, non-invasive method to measure temperature fields in analog porous media.

We employ colloids made of $\mathrm{Zr}({}^{\mathrm{Mes}}\mathrm{IPDPt}^{\text{-BuPh}})_2$, a bright and photostable zirconium(IV) complex with temperature-sensitivity exceeding 1.9%/K. The method relies on tracking the thermally activated delayed fluorescence decay of the colloids, using high-speed imaging under modulated LED excitation. The colloids' characteristic decay time depends on temperature according to a functional form that we have calibrated. The heat transport experiments consist in mixing two batches of the same aqueous solution inside an analog porous medium, with both batches containing the colloids in suspension; the resident batch initially saturating the medium is at room temperature, while the injected batch is at a controlled, higher, temperature of 50 °C. A time decay is measured for each pixel of the camera sensor, and one lifetime field is computed every 2.5 seconds, providing the temporal evolution of temperature across the pore space. The calibration curve is then used to transform that field into a temperature field, for each measurement time. The achieved temperature measurement precision, standing at ±0.3 K so far, was determined at temporal and spatial resolutions of 131 ms and 0.3 mm, respectively. The synthetic quasi-2D porous medium inside the flow cell (15 × 6 cm) is made of a material with thermal conductivity similar to that of natural aquifers. It is designed with a porosity of 0.36 and a minimum pore size of ∼0.5 mm. Varying the flow rate enables tuning the Péclet number within ranges characteristic of regimes found in natural aquifers. The experimental setup integrates a controlled injection system, type-T thermocouples at the inlet and outlet for reference temperature measurement validation, and is optically transparent to allow for the aforementioned decay time-based temperature imaging.

The resulting temperature fields reveal non-uniform thermal front propagation and spatially variable gradients, indicating conditions where Local Thermal Non-Equilibrium (LTNE) effects are significant. LTNE refers to a state where the fluid and solid phases in a porous medium maintain distinct temperatures. These patterns, not captured by point-wise measurements, highlight optical thermometry as a robust technique for capturing localized heat exchange and characterizing coupled flow and heat transport in heterogeneous porous media quantitatively, from space- and time-resolved measurements. Experimental data are compared with numerical simulations replicating porosity, grain size, and Darcy flux. Ongoing work will extend the method to other geological structures and flow regimes relevant to various hydrogeological settings.

Direct observation of calcite dissolution with microfluidics and spectral induced polarization. Geochemical and petrophysical modeling

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Keywords: microfluidics, spectral induced polarization, calcite dissolution, reactive transport modeling, petrophysical modeling

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Calcite is a very chemically reactive and common mineral in carbonate rocks like those often present in the critical zone. Its dissolution remains a physico-chemical process not completely understood at the scale of the grain and calcite dissolution effect on the measured low-frequency electrical response in geophysics is poorly known. In this study we show for the first time images of calcite grain dissolution in partially water saturation conditions from an innovative microfluidic experiment constraining a reactive transport model and a petrophysical model (Figure 1). Porosity and water conductivity were simulated. In addition to a deeper understanding of the calcite dissolution process and related electrical response due to charge carrier electromigration, our approach allows extracting from it cation exchange capacity and specific surface area, two parameters of uttermost importance in field geophysics. Our study published in [1] is a step further to understand and model the electrical response associated with mineral-water interaction at the pore scale.

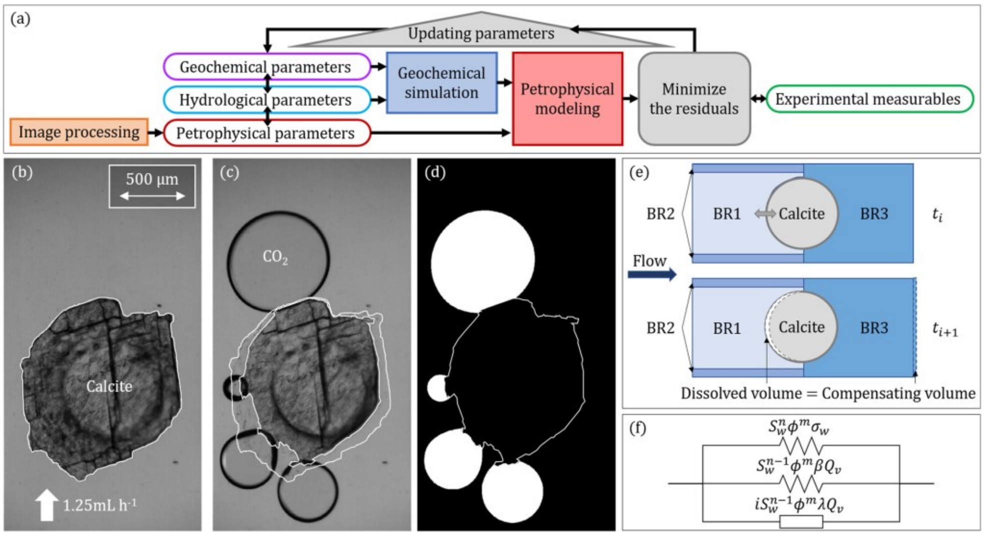

Figure 1: Approach used here to model calcite dissolution according to microfluidics imaging.

Reference

[1] F. Rembert, P. Leroy, A. Lassin, S. Roman, Microfluidics and Spectral Induced Polarization for Direct Observation and Petrophysical Modeling of Calcite Dissolution, *Geophysical Research Letters*, 51, 1-12 (2024).

Dynamic Displacement of Wetting Fluids by Non-Wetting Fluids in Geological Fractures: an Analog Experiment

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Keywords: geological fractures, two-phase flow, phase diagram

The immiscible displacement of a wetting fluid by a non-wetting fluid in rough fractures is essential for optimizing subsurface operations such as enhanced oil recovery and geological carbon sequestration (GCS). Despite its importance, a comprehensive understanding of drainage flows in fractures, considering factors such as fracture geometry, fluid properties, and flow regimes, remains elusive. To address this, we have developed an analog experimental setup featuring a transparent fracture flow cell with self-affine rough-walled surfaces, matched above a specific correlation length and with a precisely controlled mean aperture. We generate realistic synthetic fracture geometries numerically, characterized by the Hurst exponent, fracture closure, and correlation length. The fracture walls are then obtained by micro-machining of transparent PMMA plates, using those geomeries. High-speed imaging captures the dynamic spatial distribution of fluid phases between the fracture walls during drainage. We vary the mean aperture across experiments for a given fracture geometry and investigate a broad range of capillary numbers, spanning both viscous and capillary-dominated regimes, while also varying viscosity ratios to characterize resulting displacement regimes. An extended phase diagram for drainage in geological fracture is thus obtained as a function of the viscosity ratio between the two fluids, the capillary number, and the fracture aperture.

Analysis of Heat Transport in Fracture Networks with Dead-Ends

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Keywords: Heat transport, Fracture network, Dead-ended fractures

Heat transport in fractured media is characterized by coupled thermal-hydraulic (TH) processes. Hydraulic processes take place primarily within fracture networks, where the permeability and connectivity of the fractures govern fluid flow. This flow facilitates convective heat transport through the fractured medium and heat transfer between the fluid and the surrounding rock matrix, interacting with heat conduction driven by temperature gradients in both the fluid and solid matrix. Gaining insight into the interplay between these physical mechanisms and the fracture network's geometry is essential for a wide range of applications in hydrogeology and subsurface engineering. These include protecting groundwater resources, using heat as a tracer to characterize thermal and hydraulic properties of fractured sites, evaluating the heat transfer efficiency in fractured geothermal reservoirs, and assessing thermal impacts on rock properties near nuclear waste repositories.

This study extends previous research on TH processes in individual rough fractures [1], shifting the focus to fracture intersections, with particular attention to the influence of dead-ended fractures on the heat exchange between fracture and matrix. We perform numerical simulations using the OpenFOAM solver *chtMultiRegionFoam*, which models conjugate heat transfer across multiple regions. In our setup, we define two regions: a fluid region, representing the fractures in which coupled flow and heat transport occur, and a solid region, representing the impermeable rock matrix. The fluid domain is governed by the conservation equations for mass, momentum, and energy, while heat conduction alone is modeled in the solid domain.

The simulation results are analyzed using thermal breakthrough curves, the progression of the thermal front across the medium, and the heat flux across the fracture-matrix interface(s). Our findings highlight how the connectivity between fractures, fracture aperture, fracture roughness amplitude, intersection angle, and matrix thermal conductivity influence heat transport at and around fracture intersections.

References

[1] Maria Klepikova, Yves Méheust, Clément Roques, Niklas Linde, Heat transport by flow through rough rock fractures: a numerical investigation, Advances in Water Resources, 156, 104042 (2021).

Simulation Of A Porous Iron Particle Melting In A Fluid

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Keywords: Direct Reduced Iron, CFD, multiphase flows, heat transfer, mass transfer

Direct Reduced Iron (DRI) melting in an Electric Smelting Furnace (ESF) slag displays complex behaviour involving chemical reactions, heat transfer, and fluid-solid flows, resulting in rheological changes in the porous DRI matrix such as a reduction in porosity due to iron sintering [1] or slag penetration through the DRI pores [2]. This slag flows through the pore channels of the DRI, enhancing heat transfer, and consequently the melting rate, by increasing the DRI's effective thermal conductivity. If this slag originates from the bulk slag, it also contributes to an increase in particle density. The formation of slag in the pellet is also possible as its gangue melts [3]. In the case of H-DRI, the FeO, with a lower melting point, liquefies first, thus forming an autogenous slag within the DRI.

A description of local heat and mass transfer between slag and DRI is crucial for understanding the ESF process. In this work, Computational Fluid Dynamics (CFD) are used to describe the particle-scale and pore-scale melting of a single DRI particle in an ESF slag. The results are then compared to data provided by small-scale melting experiments. The final goal of this work is to obtain a representative melting model to couple with a large-scale numerical model of the ESF.

The open-source code Basilisk, a DNS code using dynamic adaptive mesh refinement following a quad/octree structure developed at Sorbonne University, is used to model the DRI melting process. The flow of air, slag, and metal is considered in the domain representing a DRI particle in a crucible of similar dimensions to the one used in the experiment. Solids and liquids are differentiated using temperature-driven properties. The temperature-dependent DRI properties are determined with in-house thermodynamic calculations. In this first approach, the DRI was represented as a homogeneous phase with apparent properties determined for a given porosity. DRI density variations were considered as resulting from bulk slag entering the pores. These flows were computed using Darcy's law inside the pellet.

This model was used to simulate the melting of a single H-DRI under conditions matching those of the experiments. The evolution of temperature distribution within the DRI matches experimental data found in the literature [4]. New simulations are to be conducted at the pore scale as the flows of air, slag and metal will be considered in the domain representing the porous matrix. This will enable a more detailed analysis of the local phenomena responsible for rheological changes, which were not accurately captured in the initial simulation.

References

[1] J. Li, M. Barati, Kinetics and mechanism of decarburization and melting of direct-reduced iron pellets in slag, *Metallurgical and Materials Transactions B*, 40, 17–24 (2009).

[2] J. Huss, A. Vickerfält, N. Kojola, The Melting Mechanism of Hydrogen Direct Reduced Iron in Liquid Slag, *Steel research international*, 95, 2300325 (2024).

[3] A. Vickerfält, J. Huss, J. Matrinsson, D. Sichen, Reaction mechanisms during melting of H-DRI focusing on slag formation and the behavior of vanadium, *Metallurgical and Materials Transactions B*, 54, 2206–2215 (2023).

[4] R.J. O'Malley, The heating and melting of metallic DRI particles in steelmaking slags, PhD Thesis, Massachusetts Institute of Technology (1983).

Improved Modelling of the Conduction-Radiation Coupling in Heterogeneous Media by a Fully Stochastic Approach

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Keywords: transient heat transfer, heterogeneous media, voxelized representation, conduction-radiation coupling, Brownian walkers, Monte Carlo ray tracing

Heterogeneous media with complex 3D morphologies have received much attention in the last decades in particular for their very interesting thermal properties. Composites, foams, or ceramics appear in many applications as insulators, heat exchangers, often for high temperature industrial applications, or as heat shields. Many numerical modelling approaches taking account of the morphological descriptions of the materials are proposed to simulate numerical experiments on their virtual representations to calculate their effective physical properties and improve them, for example by changing the nature of their components and/or the topology of their microstructure. Among them, deterministic methods such as finite differences, finite elements, or finite volumes have proved their reliability, but they found their limits when dealing with transient conduction-radiation heat transfer problems within semi-transparent complex 3D morphologies, mainly because of their massive random access memory needs. Thus, we have developed a fully stochastic approach to overcome the memory need, maybe at the price of the computation duration if the asymptotic steady state is wanted. To do so, we have coupled a Brownian walkers method for transient conduction with a Monte Carlo ray tracing method for radiation [1,2]. To avoid the complex meshing of 3D structures, especially in fibrous and porous media, our procedure uses voxelized structures directly obtained from X-ray tomographies.

During this congress, we will present the latest improvements of our approach. It concerns first the modelling of transient conduction with Brownian walkers, previously validated on moderately sized voxelized structures [1,2]. However, numerical convergence becomes challenging for high-resolution 3D porous structures due to the very large number of fluid-solid interfaces. We therefore revisit the transmission probability method and adapt it to handle strong thermophysical contrasts, introducing an interface treatment strategy based on the first hitting time [3]. The accuracy and computational cost of this new method are assessed through various test cases, and compared with other Brownian walkers interface treatments and deterministic solutions. Complementary, the Monte Carlo ray tracing method used to model radiation [2], has been adapted to account for optical index contrasts between the two phases. Reflection and refraction phenomena at interfaces are now integrated, leading to a more accurate calculation of the radiative volume heat source field and, consequently, of the resulting temperature distribution. This enhancement enables a more realistic representation of radiative transfer within heterogeneous semi-transparent materials.

References

[1] L. Seyer, V. Gonneau, F. Enguehard, D. Rochais, Improvements of the Brownian walkers method towards the modeling of conduction-radiation coupling, International Journal of Heat and Mass Transfer, 211 (2023).
[2] L. Seyer, F. Enguehard, D. Rochais, Deterministic and stochastic approaches for the modeling of conduction-radiation coupling within non-Beerian semi-transparent media, Journal of Quantitative Spectroscopy & Radiative Transfer, 325 (2024).
[3] E. Baioni, A. Lejay, G. Pichot, G. M. Porta, Random walk modeling of conductive heat transport in discontinuous media, Transport in Porous Media, 151 (2024).

Numerical simulations of turbulent flows in Double Porosity Porous Media

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Keywords: double porosity, turbulent flows, lattice Boltzmann method, TPMS

Porous media have been studied for their ability to alter flow characteristics, such as the suppression or enhancement of turbulence at various scales. For example, porous airfoils have been shown to impact the turbulent boundary layers and trailing-edge noise significantly [1]. The role of porosity, permeability, and flow geometries in shaping turbulence remains a critical area of investigation [2].

One particular aspect of porous media is the concept of *double porosity*, which can account for the dual-scale nature of flow within fractured porous media [3]. More generally, double porosity materials can be seen as porous media whose solid part is a porous material itself of lower characteristic pore size. Finding applications in hydrology [3] and acoustics [4], the turbulence properties at the pore level of flows through these types of media have yet to be unveiled, either numerically or experimentally.

This study considers a particular class of double porosity materials based on triply periodic minimal surface (TPMS) structures, characterized by their periodic, self-supported properties. The TPMS surfaces are mathematically defined by an implicit equation that requires only a few parameters. Double porosity materials incorporate a second porosity scale either by embedding micropores within the solid phase or within the interconnected voids of the macropores, see Fig. 1 below for a first result obtained in the former case using gyroid TPMS for both macro and micro pores.

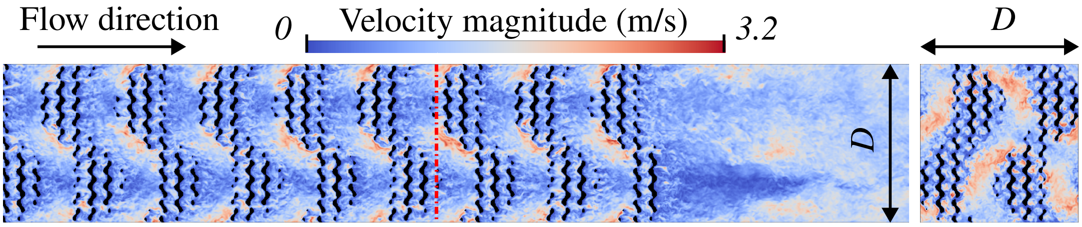

Figure 1: Longitudinal and cross-section views of the velocity field magnitude. The Red dashed line corresponds to the cross-section position.

We seek to understand how the pore topology of the two-pore networks influences large-scale turbulence behaviour. To address this, we employ the lattice Boltzmann method (LBM), a numerical approach that is particularly well-suited for simulating complex flow patterns in porous structures.

References

[1] Tamaro *et al.*, Experimental investigation of turbulent coherent structures interacting with a porous airfoil, Experiments in Fluids, 62, 94 (2021)

[2] Jin *et al.*, Numerical investigation of the possibility of macroscopic turbulence in porous media: a direct numerical simulation study, Journal of Fluid Mechanics, 766, 76-103 (2015)

[3] Ma *et al.*, Constitutive Modeling of Hydromechanical Coupling in Double Porosity Media Based on Mixture Coupling Theory, International Journal of Geomechanics, 23, 6 (2023)

[4] Olny *et al.*, Acoustic wave propagation in double porosity media, The Journal of the Acoustical Society of America, 114, 73-89 (2003)

Texture-based assessment of gas adsorption selectivity on porous carbons with enhanced separation properties

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Keywords: Gas separation, textural characterization, molecular sieves

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Typical separation of carbon dioxide from flue gas or methane from biogas (i.e. CO_2/N_2 and CH_4/CO_2 separation respectively) can be achieved using, for example, Pressure Swing Adsorption (PSA) units which contain adsorbent beds. A thermodynamic (adsorption) and kinetic (diffusion) separation of the molecules contained in the feed gas is then carried out within the adsorbent bed. It is the reason why the assessment of gas adsorption selectivity (i.e. thermodynamic part of the separation) of activated carbons (ACs) and carbon molecular sieves (CMS) is a preliminary and necessary step for the design of such PSA units. Nevertheless, the adsorption of the gas of interest can be dangerous (e.g. CH_4) at laboratory scale. As consequence, the calculation of the gas adsorption selectivity at near zero coverage (S_0) based on the sole textural properties can be considered to be a convenient tool in order to avoid such safety-related constraints and to carry out a rapid selection of potential carbon molecular sieves. The calculation of S_0 is based on the previously obtained pore size distributions (PSDs). The latter ones were obtained using different methods (i.e. NLDFT or GCMC-based isotherms kernels **[1, 2]**). Subsequently, a simple calculation based on the Steele potential **[3]** and combined to such PSDs allowed the calculation of Henry constants ($K_H(CO_2)$, K_H (N_2) and K_H (CH_4)) for each gas on several porous carbons. S_0 was then approximated by the ratio of these henry constants (e.g. $S_0(CO_2/N_2) = K_H(CO_2)/K_H(N_2)$) (***figure 1.a***). In addition, a way a synthesis combining sol-gel, soft-templating and hydrothermal treatment was implemented in order to produce enhanced CMS (***figure 1.b***). Surprisingly, the lab-maid CMS exhibited higher selectivity than their commercial counterparts (***figure 1.a*** in pink). These results can be explained by the high degree of crosslinking of the polymer precursor and, as a consequence, of the extremely narrow character of the resulting pores of the carbon matrixes (***figure 1.b***).

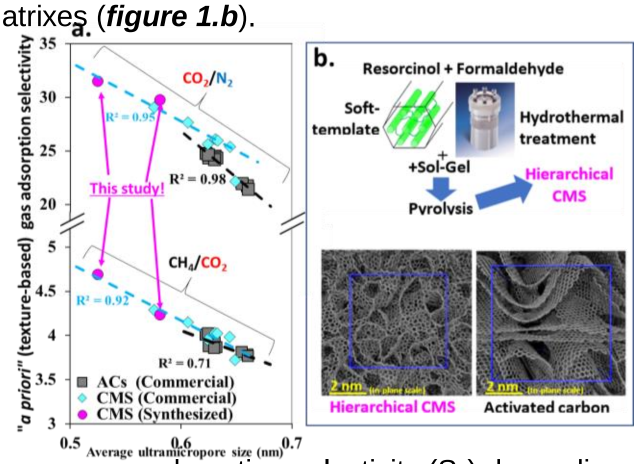

Figure 1: **a.** Near zero coverage adsorption selectivity (S_0) depending on ultramicropores size, **b.** simplified methodology of CMS synthesis and structural reconstruction of the ACs and CMS.

References: **[1]** J. Jagiello and J. P. Olivier, "2D-NLDFT adsorption models for carbon slit-shaped pores with surface energetical heterogeneity and geometrical corrugation," Carbon, vol. 55, pp. 70-80, Apr 2013, **[2]** F. Vallejos-Burgos et al., "3D nanostructure prediction of porous carbons via gas adsorption," Carbon, vol. 215, Nov 2023, Art no. 118431, **[3]** W. A. Steele, "Physical interaction of gases with crystalline solids .1. gas-solid energies and properties of isolated adsorbed atoms," Surface Science, vol. 36, no. 1, pp. 317-352, 1973 1973

Carbonization Kinetics and Textural Properties of Activated Carbons Derived from the hulls of *Lophira lanceolata*

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Keywords: Activated carbons, kinetic modeling, textural Properties

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Abstract: This study explores the thermochemical elaboration and characterization of activated carbons derived from *Lophira lanceolata* hulls. The process includes conditioning, an alkaline pretreatment with NaOH, impregnation with phosphoric acid (H_3PO_4) at various ratios, followed by activation/pyrolysis at 500°C for 2 hours [1]. A final Soxhlet washing step removes mineral ash and enhances porosity. The kinetic modeling of activation/pyrolysis is based on a four-step multi-reaction model, integrating Arrhenius' law to estimate mass fractions, kinetic constants, and activation energy [2]. The simulation model is validated by its close correlation with experimental data and the low error function values, demonstrating its precision and reliability. Textural analysis, performed via nitrogen (77K) and CO_2 (273K) adsorption using BET and 2D-NLDFT models, highlights a micro-mesoporous structure [3]. Specific surface areas range from 1850 to 2139 $m^2.g^{-1}$ (BET) and 1543 to 1812 $m^2.g^{-1}$ (2D-NLDFT). Pore distribution analysis reveals ultramicropores (~6Å) and expanded porosity (>50Å) at higher impregnation ratios. These results underscore the potential of the obtained activated carbons for advanced adsorption applications.

References

[1] Elie Sogbochi, Pierre Girods, Guevara Nonviho, Sebastien Fontana, Yann Rogaume, Dominique Codjo Koko Sohounhloue, Use of Carbonaceous Materials Derived from Co-products of *Lophira lanceolata* for Adsorption Tests of Congo Red Dye, *American Journal of Physical Chemistry*, **11**(4), 91-101(2022). doi: *10.11648/j.ajpc.20221104.12*

[2] Elie Sogbochi, *Elaboration par voies thermochimiques de charbons actifs dérivés de coproduits de Lophira lanceolata : essais d'adsorption de micropolluants de l'eau.* Thèse de doctorat en cotutelle internationale entre l'Université d'Abomey-Calavi (UAC/Bénin) et l'Université de Lorraine (UL/France). P.292 (2023) *https://theses.fr/api/v1/document/2023LORR0194*

[3] Elie Sogbochi, Clement Kolawolé Balogoun, Guevara Nonviho, Saka Moussiliou, Cokou Pascal Agbangnan Dossa, Dominique Codjo Koko Sohounhloue, Synthesis of porous carbons for the fixing of cationic molecules in aqueous solution, *Scientific African*, **25**, e02332(2024). https://doi.org/10.1016/j.sciaf.2024.e02332

Mixing in confined heterogeneous porous media

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Keywords: Mixing, Porous Media, Transport Phenomena

Solutes mixing by porous media flows is the result of complex transport phenomena that controls natural and industrial systems. Despite the relevance of mixing, the impact of the microscopic (pore-scale) controlling mechanisms under confinement are not yet fully understood. The main challenge is the upscaling of mixing confinement: the microscopic quantities that characterise such condition are two-fold: i) no-slip (for flow) and no-flux (for solute transport) at solid grain walls. To address this, we performed numerical simulations and laboratory experiments based on microfluidics and time-lapse video microscopy. These complementary datasets allow us to capture detailed spatial-temporal evolution of diagnostic parameters which quantify mixing, such as scalar dissipation rate, concentration and gradients statistical distributions (PDF). These findings highlight the impact of a pore structure, and the associated confinement, on macroscopic mixing in porous media.

Measurements of concentration gradients in geological porous media using microfluidic devices and Raman spectroscopy

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*Keywords: c*oncentration gradients, diffusiophoresis, microfluidics, Raman spectroscopy

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 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 porous media using conventional mechanisms such as pressure gradients or gravity is challenging. By establishing a solute concentration gradient within pores, it is possible to induce a flow of particles into or out of the pores under controlled conditions [1]. This phenomenon is known as diffusiophoresis. In geological formations, local concentration gradients arise from a number of physicochemical processes, such as salt or crystal dissolution, drying, precipitation, interphase mass transfer, and chemical reactions. However, it remains unclear whether such local chemical gradients are sufficient to induce diffusiophoretic transport of colloidal particles.

The present study assesses the magnitude and spatial distribution of local concentration gradients generated *in situ* during mineral dissolution, and evaluate their potential to deliver colloidal particles to regions of interest. We have developed an experimental approach that combines microfluidics and Raman spectroscopy. Thanks to transparent micromodels, microfluidic devices allow direct visualization of flows and reactions at the pore-scale. Raman spectroscopy is a non-invasive and non-destructive technique used for *in situ* monitoring of structural and chemical changes during a reaction [2]. Althought Raman scattering is commonly used for studying mineralogical evolution, only a few studies are devoted to detect species in solutions. First, our methodology has been applied to study calcite dissolution, a common reaction in geological environments, in real time under static and dynamic conditions. Analysis of Raman spectra allowed identifying the chemical species involved in the dissolution process. Thus, it provides new insights into the hydrogeochemical couplings involved in geological environments. The outcomes aim to contribute to our understanding of local concentration gradients in geological porous media, paving the way for improved predictions and management of subsurface processes.

References

[1] S. Roman et al. Physical Review Fluids, 10(3):L032501, 2025.
[2] J. Poonoosamy et al. Lab on Chip, 20(14):2562, 2020.

X-Ray Based Structural Characterization Of A Ceramic Microfiltration Membrane For LBM Simulations

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Keywords: X-ray tomography, 3D reconstruction, Lattice-Boltzmann method

Ceramic microfiltration membranes are widely used due to their excellent mechanical, chemical and thermal stability. However, their potential is limited by fouling, making it necessary to clean the membranes after some usage time. The highly complex fouling mechanisms remain poorly understood, especially in the membrane's internal structure and regarding their dependence on structural characteristics such as tortuosity and interconnectivity [1].

To comprehend these mechanisms and optimize chemical or backwashing processes, a detailed structural analysis of the membrane is essential. While many characterization techniques are either destructive or limited to surface analysis, X-ray micro- and nano-tomography provide non-destructive, 3D imaging of both the membrane's skin layer and its support structure, including the structural transition between them.

We acquired microtomography data of the membrane support and reconstructed the 3D model of the sample. Figure 1 shows a raw grey-level tomography image and the final binarized 3D reconstruction. Key parameters such as porosity variation and pore and throat size distribution were analyzed in iMorph, using granulometry and the maximum ball algorithm [2].

The skin layer was studied by combining absorption and phase-contrast nano-tomography.

The porosity of each structure was compared with values from complementary measurements. Beyond structural insights, the reconstructed volumes serve as realistic input for Lattice-Boltzmann simulations. These fluid flow simulations will enhance the understanding of constriction structures and fouling mechanisms, contributing to the development of more effective backflush strategies.

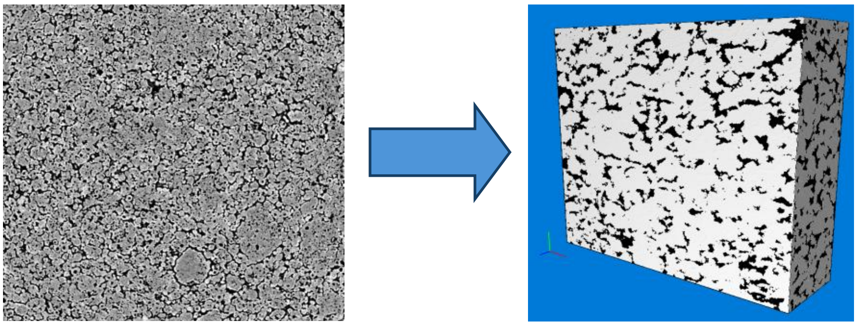

Figure 1: By binarizing the raw 2D slices (left), the 3D volume of the membrane structure is reconstructed (right).

References

[1] Bacchin, P., Derekx, Q., Veyret, D., Glucina, K., & Moulin, P., Clogging of microporous channels networks: role of connectivity and tortuosity, *Microfluidics and Nanofluidics*, 17, 85-96, (2014).

[2] Mathilda Trevisan, Jérôme Vicente, Rémy Ghidossi, Adrien Vincent, Philippe Moulin, Membrane characterisation from the support to the skin layer: Application to silicon carbide (SiC) membranes, *Journal of the European Ceramic Society*, 42, 3759-3769 (2022).

A THMC Approach For Crack Appearance Within Reactive Porous Media Under Hydrochemo-Mechanical Loads

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Keywords: reactive transport, chemo-mechanical coupling, cement carbonation

Coupled Thermal-Hydraulic-Mechanical-Chemical (THMC) approaches are crucial for a wide range of engineering and geosciences applications. Hence, their development have been the subject of numerous research projects over the past 20 years. However, due to the intrinsic complexity associated to simultaneously describe flow, species transport, chemical and mechanical effects together, no thorough dynamic two-way feedback between these processes have yielded satisfactory results. We present a novel approach to overcome past limitations by coupling two state-of-the-art simulators. Our numerical approach rests on a sequential non iterative coupling between Hytec, a reactive transport algorithm and Cast3M, a mechanical code. Hytec computes the evolution of hydraulic and mineralogical fields allowing to compute the micromechanical properties (e.g. Young modulus). The mineral reactions and drying processes generate tensile stresses and change in capillary pressure. Cast3M computes the associated strain tensors and induced damage. The damage model allows to account for the evolution of a crack network whose transport properties are computed based on the crack apertures. In the case of crack appearance, Cast3M thus imposes the increase of a double porosity in Hytec, which accelerates the subsequent reactive transport processes. We validate our method on the accelerated unsaturated carbonation of cementitious materials by comparing the predicted crack network and degradation depths with microtomographic images. We demonstrate that the shape of the degradation front results from the coupled impacts of chemistry and mechanics together. Based on its physical basis, our approach can be extended to different hydro-chemo-mechanical loadings.

References

[1] Socié, A., Seigneur, N., Bary, B., Poyet, S., & Touzé, G. A fully coupled Hydraulic Mechanical Chemical approach applied to cementitious material damage due to carbonation. *Npj materials degradation*, *7*(1), 60 (2023).

Exploring Water Transport and Aging Mechanisms in Bio-Based Porous Materials through NMR Relaxometry

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Keywords: Aluminosilicate hydrogels; NMR relaxometry; water dynamics; sustainable construction; green chemistry; agriculture; zeolites; bio-based materials; soil stabilization; porous media.

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.

References

[1] Poulesquen, A.; Gomes Rodrigues, D.; Keshavarz, B.; Courtois, N.; Ilavsky, J.; McKinley, G.; Aluminosilicate colloidal gels: from the early age to the precipitation of zeolite; Soft Matter; 20 (2024).

[2] Maillet, B.; Sidi-Boulenouar, R.; Coussot, P.; Dynamic NMR Relaxometry as a Simple Tool for Measuring Liquid Transfers and Characterizing Surface and Structure Evolution in Porous Media; Langmuir; 38, 15009–15025 (2022).

Disorder-induced non-linear growth of fingers during immiscible two-phase flow in porous media

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Keywords: two-phase flow, viscous instability, non-Darcian flow

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Immiscible two-phase flow in porous media produces different types of patterns depending on the capillary number *Ca* and viscosity ratio *M*. At high *Ca*, viscous instability of the fluid–fluid interface occurs when the displaced fluid is the more viscous, and leads to viscous fingering, which is believed to exhibit the same growth behavior as the viscously-unstable fingers observed in Hele–Shaw cells by Saffman and Taylor in their seminarl study [1], or as diffusion-limited aggregates (DLA). In such Laplacian growth processes, the interface velocity depends linearly on the local gradient of the physical field that drives the growth process (for two-phase flow, the pressure field). However, a non-linear power-law dependence between the flow rate and the global pressure drop, reminiscent of what has also been observed for steady-state two-phase flow in porous media, was evidenced experimentally for the growth of viscously-unstable drainage fingers in two-dimensional porous media, 20 years ago. Here, we revisit this flow regime using dynamic pore-network modeling and explore the non-linearity in the growth properties. We characterize the previously unstudied dependencies of the statistical finger width and non-linear growth law's exponent on Ca [2], and discuss quantitatively, based on theoretical arguments, how disorder in the capillary barriers controls the growth process' non-linearity [2], and why the flow regime crosses over to Laplacian growth at sufficiently high Ca. In addition, the statistical properties of the fingering patterns are compared to those of Saffman–Taylor fingers, DLA growth patterns, and the results from the aforementioned previous experimental study.

References

[1] P. G. Saffman, G. I. Taylor (1958), The penetration of a fluid into a porous medium or Hele–Shaw cell containing a more viscous liquid, Proc. R. Soc. London 245, 312

[2] S. Sinha, Y. Méheust, H. Fyhn, S. Roy, A. Hansen (2024), Disorder-induced non-linear growth of fingers in immiscible two-phase flow in porous media, *Phys. Fluids* **36**, 033309.

Modeling Complex Flows In Porous Media With ComPASS.

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Keywords: flows in porous media, multi-phase, multi-component, thermal flow, discrete fracture network

ComPASS [1] is an open-source, massively parallel simulator for multi-phase, multi-component flow, designed with a mixed-dimensional approach to accurately model 3D porous media, 2D fractures, and 1D wells. All domains are discretized on a shared unstructured (typically polyhedral) mesh: porous media are represented by mesh elements (3D), fractures by mesh faces (2D), and wells by mesh edges (1D). Modeling of underground systems strongly benefits from the use of unstructured meshes since the latter can handle arbitrary geometries. Spatial discretization is based on the Vertex Approximate Gradient (VAG) finite volume scheme, a scheme designed to be very efficient (accuracy *vs* number of degrees of freedom) on polyhedral meshes. Moreover, this scheme has been carefully adapted to enable robust coupling between the mixed-dimensional features.

Initially developed for simulating complex geothermal systems [2], ComPASS has since been extended to applications in hydrology and gas storage. Ongoing developments aim to integrate additional physical processes, such as geomechanics and chemical reactivity, further enhancing the simulator's capabilities.

References

[1] https://gitlab.com/compass
[2] A. Armandine Les Landes, L. Beaude, D. Castanon Quiroz, L. Jeannin, S. Lopez, et al., Geothermal modeling in complex geological systems with ComPASS. Computers Geosciences, 194, pp.105752 (2025)

NH_3-responsive chromism of cyanine dyes adsorbed on surface-modified mesoporous silica

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Keywords: Mesoporous Materials, Molecular responsive chromism, Optical sensor

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In chromic materials with high substrate selectivity (molecular recognition ability) based on organic crystals or MOFs[1], the structure of the functional group of the materials, the interactions between the functional group and the substrate and/or the crystal structure of the materials change in response to the substrate adsorption, causing a change in the electronic state that results in chromism. Materials with high substrate selectivity require a precise design and synthesis of a structure that corresponds well to the target substrate.

As a model example that can be easily synthesized in comparison with those with higher selectivity, I will present the synthesis of substrate-responsive chromic materials by placing a dye, which does not show substrate responsiveness by itself, in a nanospace: a cationic cyanine dye (1,1'-Diethyl-2,2'-cyanine; PIC) was adsorbed on a mesoporous silica thin film[2] modified with propylsulfonic acid groups. When ammonia gas was passed through this film, an absorption band at around 570 nm, assigned to J-aggregates[3], appeared. When air was passed through, the absorption spectrum returned to its initial one. This is thought to occur because ammonia was adsorbed to the sulfonic acid groups, causing the cationic PIC, which initially interacted electrostatically with the sulfonic acid groups, to be temporarily displaced and aggregated.

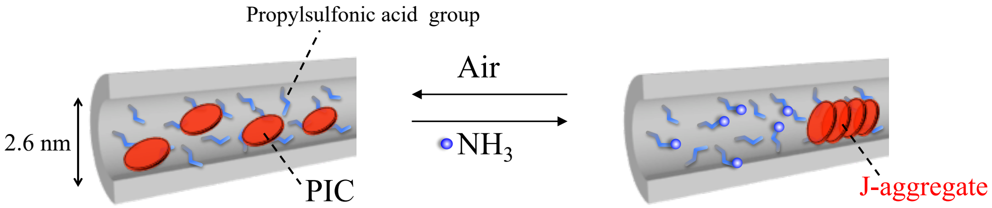

Figure 1: Schematic drawing of ammonia-responsive chromism of PIC-adsorbed surface-modified mesoporous silica film.

References

[1] Y. Shen, A. Tissot, C. Serre. *Chem. Sci.*, 13, 13978 (2022).
[2] N. Shimura, M. Ogawa, *J. Colloid Interface Sci.*, 312, 311 (2007).
[3] B. Kopainsky, J. K. Hallermeier, W. *Kaiser, Chem. Phys. Lett.* 83, 498 (1981).

Radiative Characterization of a Fibrous Medium by Cylinder Stack Morphological Study and Monte Carlo Method

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Keywords: Radiative transfer, Fibrous medium, Monte Carlo method

Thermal insulation at high temperatures relies most of the time on highly porous materials made of fibers or particles of small spatial dimensions. In these materials, the radiative transfer plays a key role that must be characterized at all scales.

In this work, we study a stack of possibly overlapping infinite cylinders under vacuum, assumed to be representative of a real fibrous medium. The solid phase is assimilated to a homogeneous cold dense participating medium, absorbing but non-scattering, characterized by its spectral complex optical index. The distribution of cylinders inside the calculation box is chosen to be statistically homogeneous and isotropic to ensure interesting morphological properties. To achieve this, an algorithm [1] generates each cylinder axis as a µ-random chord [2] of the calculation box. Analytical expressions for the average porosity and various phase correlation functions can be deduced.

To simulate the propagation of radiation inside the box, a Monte Carlo ray tracing method is implemented. Each ray enters the box following a direction that complies with the conditions of the incident illumination, and may be absorbed inside the cylinders, or reflected or refracted at the interfaces between the cylinders and the vacuum. The fractions of rays exiting the box provide the reflectance (R) and transmittance (T) values of the calculation domain. The radiative properties of the equivalent homogeneous medium are then determined by inversion of these results using the least squares method, by comparing them with an absorbing-scattering flat wall model with either isotropic, Henyey-Greenstein or arbitrary Legendre series scattering phase functions. A procedure for computing parameters sensitivities in each scenario and despite the statistical noise intrinsic to the Monte Carlo method is shown [3].

Results obtained for a large value of the porosity seem acceptable for different scattering phase functions. On the other hand, further calculations carried out for a lower value of the porosity lead us to question the validity of our model. Moreover, there is a real difficulty in carrying the inversion with Legendre series due to strong parameters constraints. Some areas for further study are suggested, among which accounting for the non-Beerian behavior of the fiber phase [4]. The possibility of determining the chord length distribution of the fiber phase is also in progress [5].

References

[1] E. Marakis and al, Uniform line fillings, *Physical Review E* 99 (2019)
[2] R. Coleman, Random paths through convex bodies, *Journal of Applied Probability* 6, pp. 430-441 (1969)
[3] De Lataillade and al, Monte Carlo method and sensitivity estimations. *Journal of Quantitative Spectroscopy and Radiative Transfer* 75, 529–538 (2002)
[4] M. Tancrez, J. Taine, Direct identification of absorption and scattering coefficients and phase function of a porous medium by a Monte Carlo technique, *International Journal of Heat and Mass Transfer*, 47(2), 373-383 (2004)
[5] B. Lu and S. Torquato, Chord length and free path distribution functions for many body systems, *Journal of Chemical Physics* 98, pp. 6472-6482 (1993)

Benchmark Exercise on the Numerical Prediction of Permeability of Anisotropic Fibrous Materials

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Keywords: anisotropic porous materials, permeability, numerical modelling

In manufacturing processes of composite materials, where a reinforcing fibrous preform is impregnated with a liquid resin, a key parameter for the impregnation of reinforcements is their permeability. Experimental measurements of permeability of composite reinforcements are time-consuming and require specialized equipment. A benchmark exercise devoted to the numerical characterization of permeability was organized as a promising alternative for the determination of this parameter.

Multiple studies have been carried out in the field of numerical prediction of saturated permeability in recent years. However, there is no currently well-established methodology. This was confirmed by a large variety of approaches used in the first stage of the Virtual Permeability Benchmark [1]. The main concept of this benchmark study is to perform the computations based on real 3D images of fibrous composite reinforcements, which allows to address an important feature of this class of materials – their high variability. While this approach was applied to other classes of porous media, this benchmark exercise is the first contribution to the real fibrous materials.

The first stage of the benchmark consisted in the prediction of permeability at the scale of fibres. The focus of the second stage is the permeability computation at the scale of textiles, which are composed of tows themselves composed of fibres. The permeability of tows computed in the first stage served as an input for meso-scale calculations of flow through the textile to predict its mesoscopic permeability.

As both stages of the benchmark use the same material from the experimental permeability benchmark [2], the numerical prediction results can be compared to experimental measurements at the corresponding fibre volume fraction. A global fibre volume fraction of ~54% (porosity of 46%) was chosen. For this fibre content the presence of a non-negligible flow at both scales – inter-tow and intra-tow – is expected. It allowed thus to investigate the potential of multi-scale approaches.

Outcomes from the two stages of the Virtual Permeability Benchmark, which involved in total 21 participants from 11 countries, will be presented in details in this talk.

References

[1] Syerko E., Schmidt T., May D., Binetruy C., Advani S.G. et al. Benchmark Exercise on Image-Based Permeability Determination of Engineering Textiles: Microscale Predictions. *Compos. Part A Appl. Sci. Manuf.*, 167, 107397 (2023).

[2] May D., Aktas A., Advani S.G., Berg D.C., Endruweit A. et al. In-plane Permeability Characterization of Engineering Textiles Based on Radial Flow Experiments: A Benchmark Exercise. *Compos. Part A Appl. Sci. Manuf.*, 121, 100-14 (2019).

Poiseuille flow for S-shaped shear-thickening fluids : streamwise banding and viscous sandglasses

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Keywords: Shear thickening fluids, Poiseuille flow, Heterogeneous porous media

Shear thickening fluids exhibit complex rheological behaviour, especially when subjected to varying stress conditions. This study investigates the non-monotonic, S-shaped rheology of cornstarch in Poiseuille flow using an integrated approach of experimental measurements and numerical simulations within the Wyart-Cates rheological model framework. Using a capillary rheometer and 2D Lattice Boltzmann simulations, we observe a unique flow curve characterised by a maximum-jump-plateau behaviour : the flow rate increases monotonically to a peak and then decreases abruptly to an almost constant rate over a wide range of flow rates. By developing a dynamical stochastic version of the Wyart-Cates model, we explore the intricate mechanisms underlying this flow behaviour, with particular emphasis on the possible emergence of streamwise pressure gradient banding and the formation of high-viscosity 'sandglass' structures. Our results show that the final state of the fluid is highly sensitive to its initial homogeneity, and that the mere presence of a non-monotonic rheological curve can predict streamwise stress banding. We then investigate the flow properties of such a fluid in heterogeneous porous media. Here the flow is strongly restrained by the presence of such viscous sand glasses within the heterogeneous porous structure.

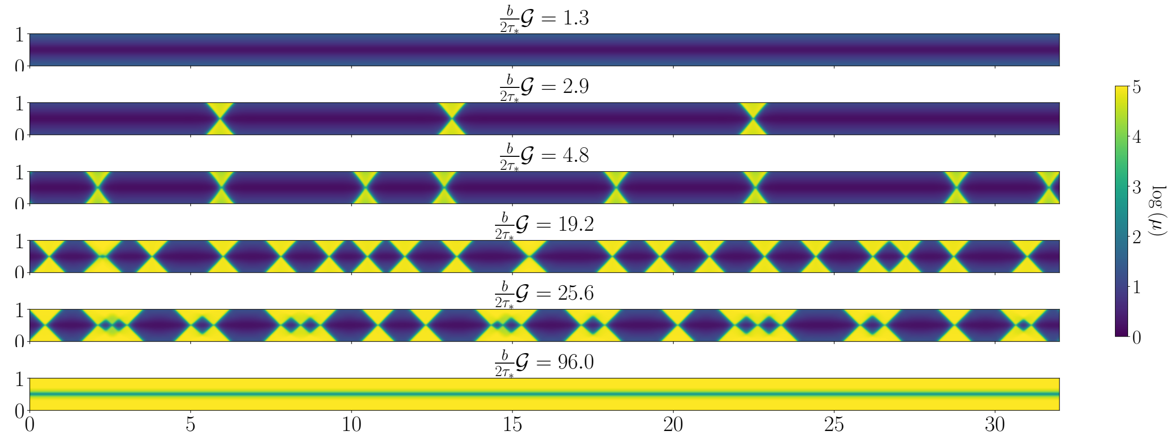

FIGURE 1: Viscosity distribution from the numerical simulations for $M = 300$ and different pressure drop.

Clayrock electrokinetic coupling modelling using LBM

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Keywords: Lattice Boltzmann Method (LBM), Electrokinetic coupling, Clayrock

A full understanding of the migration behavior of corrosion gases in clayrocks is of fundamental importance for the reliability of scenarios predicting the long-term safety of geological repositories. The Callovo-Oxfordian (COx) clayrock, studied in France as a potential host rock, exhibits a pore size distribution predominantly mesoscopic (nm), where different processes occur and interplay. The complex multiphysics couplings involved in these nanoscopic environments lead to a strongly coupled and nonlinear evolution of effective properties such as diffusion or relative permeability. Among these mechanisms, electrokinetic coupling, is likely to significantly influence how gas is transported through the rock, and by extrapolation, how radionuclides are transported. Indeed, the displacement of the alkaline disturbance generates an electrostatic field [1].The impact of pore-scale evolutions of the electrostatic potential field in clayrocks, in particular on fluid velocity and ions concentration fields is an area of interest [2].

At the pore scale, electrokinetic coupling can be modeled by combining the Stokes equation with the Poisson and Nernst-Planck equations (PNP model). The present work uses a Lattice Boltzmann model for the set of equations inspired by [3]. Different flow conditions will be first investigated for a 2D isolated pore using a set of parameters representative of the COx formation or within a range of estimated values for least known properties (e.g. surface charge density). Our study revealed that the results are independent of the ionic concentration of the solvent at low surface charge densities. The latter is more critical, as the system's behavior changes more drastically: a high surface charge density significantly reduces the thickness of the electrical double layer and alters the velocity field profile within the channel.

This model is then applied to a 2D nanoporous medium constructed from FIB-SEM images of recompacted illite, and a comparison with and without electrokinetic coupling is carried out.

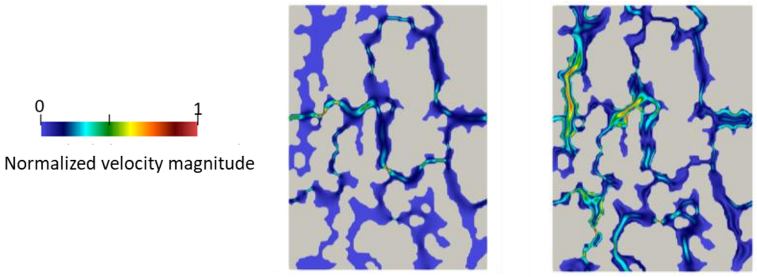

Figure 1: Velocity fields without (left) and with (right) electrokinetic coupling.

References

[1] ANDRA, Dossier 2005 Argile: Evolution phénoménologique du stockage géologique, *in Collection Les Rapports*, 2005, p. 520 (2005).

[2] C. Tournassat et C. I. Steefel, Reactive Transport Modeling of Coupled Processes in Nanoporous Media, in *Reviews in Mineralogy and Geochemistry*, vol. 85, Mineralogical Society of America, p. 75- 109 (2019)

[3] H. Yoshida, T. Kinjo, et H. Washizu, « Coupled lattice Boltzmann method for simulating electrokinetic flows: A localized scheme for the Nernst-Plank model », Commun. Nonlinear Sci. Numer. Simul., vol. 19, no 10, p. 3570- 3590 (2014)

Multiscale reactive transport modeling of ion transport in charged porous media

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Keywords: reactive transport modelling, Crunch, Poisson-Nernst-Planck, clay, electrostatics

Natural and engineered barrier systems often consist of multiple materials that are typically distributed in complex 3D geometries. Each of the materials requires its own set of process models to describe the migration of contaminants and the changes in time-dependent properties. Add to this the fact that the processes themselves are often coupled (e.g., heat, mechanical, hydrological, and chemical [THMC] coupling), and the challenge begins to look daunting. Reactive transport software has been crucial to understanding these coupled processes, yet the majority of models often do not address a number of important challenges. A particular challenge associated with geological repositories that is only rarely addressed is that of charged porous media, such as clay materials. where ion mobility is not merely a function of concentration gradients but is also influenced by electrostatic interactions. In clay environments, electrostatic interactions are most often omitted in predictive reactive transport modeling (RTM) simulations, in contrast with their acknowledged critical effects on the adsorption and transport of contaminants such as radionuclides. The challenge of capturing the electrostatic effects on ion migration in natural (clay rock) and engineered (bentonite) materials also presents a substantial computational challenge, particularly when playing out over larger repository length scales and 3D geometries. In addition, reactive transport codes often do not consider the inherently multiscale nature of the problem, with processes occurring at the millimeter (or less) scale affecting both near-field and far-field migration of radionuclides into the biosphere. The relatively large size of repository systems and their multiscale nature call for high-performance computing at the leading edge of what is possible today. Given these complexities, it is critical to apply a new generation of modeling tools capable of capturing reactive transport phenomena over large spatial and temporal scales. We will present the most recent developments of CrunchODiTi, a massively parallelized reactive transport code, evolved as part of the Crunch family of codes, able to model natively three-dimensional solute migration with off-diagonal coupled processes related to electrostatic forces in multiporosity domains and from nanometer to field scale.

Numerical Study of Reactive Transport in Unsaturated Porous Media

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Keywords: reactive transport, unsaturated porous media, surface reactions

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Reactive transport in porous media plays a fundamental role in a broad spectrum of natural and engineered systems. This process usually involves a complex coupling between hydrodynamic transport and chemical reactions, including advection, dispersion, chaotic mixing, adsorption, and various reaction mechanisms [1]. Under unsaturated conditions, the coexistence of immiscible fluid phases-typically air and water-adds significant complexity, giving rise to capillary effects, preferential flow pathways, and discontinuous fluid clusters that fundamentally alter solute transport and reaction environments. Despite their importance, the pore-scale mechanisms that govern reactive dynamics under partially saturated conditions remain not well understood. In particular, the presence of disconnected air clusters can enhance flow heterogeneity, limit mixing, and introduce non-trivial spatial variations in solute residence, which in turn influence the extent and rate of chemical reactions [2].

In this study, we investigate reactive transport process in porous media using numerical modeling. The steady-state flow field in the liquid phase is computed by solving the Stokes equations in a quasi-2D porous medium composed of cylindrical solid structures, while accounting for geometric effects associated with the third dimension. Solute transport is modeled using a Lagrangian Random Walk Particle Tracking (RWPT) framework. Surface reactions are incorporated through a collision-based approach that allows for the implementation of arbitrary nonlinear reaction kinetics [3]. This framework enables the study of a wide range of surface-mediated reactions relevant to subsurface systems, such as mineral dissolution at fluid-solid interfaces, as well as PFAS adsorption at gas-liquid interfaces. By examining solute transport and reaction dynamics under both saturated and unsaturated conditions, we aim to deepen the understanding of how air clusters and fluid phase configurations affect mixing, dispersion, and surface reactivity. The insights gained from this work could contribute to the development of improved predictive models for reactive transport in variably saturated porous media, with potential applications in contaminant attenuation, nutrient transformation, and emerging challenges such as PFAS contaminants in the vadose zone.

References

[1] Dentz M, Le Borgne T, Englert A, et al. Mixing, spreading and reaction in heterogeneous media: A brief review[J]. Journal of contaminant hydrology, 2011, 120: 1-17.

[2] Markale I, Velásquez-Parra A, Alcolea A, et al. Mixing controlled adsorption at the liquid-solid interfaces in unsaturated porous media[J]. Transport in Porous Media, 2023, 146(1): 159-175.

[3] Aquino T. Coupled nonlinear surface reactions in random walk particle tracking[J]. Advances in Water Resources, 2024, 185: 104656.

Pore-Scale Study of Pickering Emulsions for Chlorinated Solvent Remediation via Compositional Ripening

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Keywords: soil remediation, Pickering emulsion, compositional ripening, microfluidics.

Chlorinated organic compounds (COCs) are known for their environmental persistence, toxicity, and poor solubility in groundwater, making them a significant source of secondary contamination [1, 2]. Since the late 1970s, zero-valent iron (ZVI) has been explored as a remediation agent for COCs [3]. The nanoscale form of ZVI (nZVI) offers enhanced reactivity primarily due to its increased specific surface area, which provides more active reaction sites. Despite this, nZVI suffer from several drawbacks such as rapid oxidation and aggregation, both of which reduce their surface area, reactivity, and mobility [4]. To address these limitations, this study explores the use of Pickering emulsions as a novel carrier system to encapsulate nZVI. This method not only protects nZVI from premature oxidation but also enhances their transport through porous media. Pickering emulsions have previously demonstrated effectiveness in physical remediation applications [5]. Our research focuses on characterizing the flow behavior of these emulsions, fluid-phase interactions, and trichloroethylene (TCE) removal mechanisms using precisely controlled pore-scale experiments in microfluidic devices.The experiments were conducted using a water-wet microchip with pore widths ranging from 4 to 440 µm and a uniform depth of 20 µm. The chip had a porosity of 0.52 and an absolute permeability of 2.5 Darcy. Emulsions were prepared with rapeseed oil as the dispersed phase, containing silica nanoparticles (2.5 wt%) as stabilizers. Surface modification of silica particles was achieved using tetradecyltrimethylammonium bromide (TTAB, 0.027 wt%) in the continuous phase. TCE was dyed for visualization and brought to residual oil saturation (S_{or}) following the emulsion flooding. The experimental process included water saturation, TCE drainage, water imbibition and emulsion flooding. Figure 1 presents the images of each experimental procedure. S_{or} variations were tracked over time at static conditions using microscopy and image processing via ImageJ.

The results demonstrate that emulsion flooding with a volume fraction (ϕ) of 0.1 led to effective physical displacement, resulting in a residual oil saturation (S_{or}) of 19% (Figure 1). After injection, the flow was stopped, and the system was left under static conditions for 24 hours to observe subsequent changes (Figure 2a). High-magnification imaging over the first 15 hours showed an increase in droplet size along with a gradual decrease in the volume of trapped TCE, attributed to compositional ripening (Figure 2b). During this process, TCE migrated from the continuous phase into the emulsion droplets. This led to the transfer of up to 85% of the initially trapped TCE in the residual ganglia into the droplets, potentially improving contact with later-introduced nZVI and initiating degradation. Ongoing gas chromatography analyses are being conducted to confirm the extent of TCE reduction. In summary, this study highlights the potential of Pickering emulsions as a dual-function platform for in-situ remediation, enabling both efficient physical displacement and enhanced mass transfer of chlorinated solvents via compositional ripening. The findings offer new insights into pore-scale transport dynamics and establish a foundation for advanced remediation strategies that integrate physical and chemical removal mechanisms.

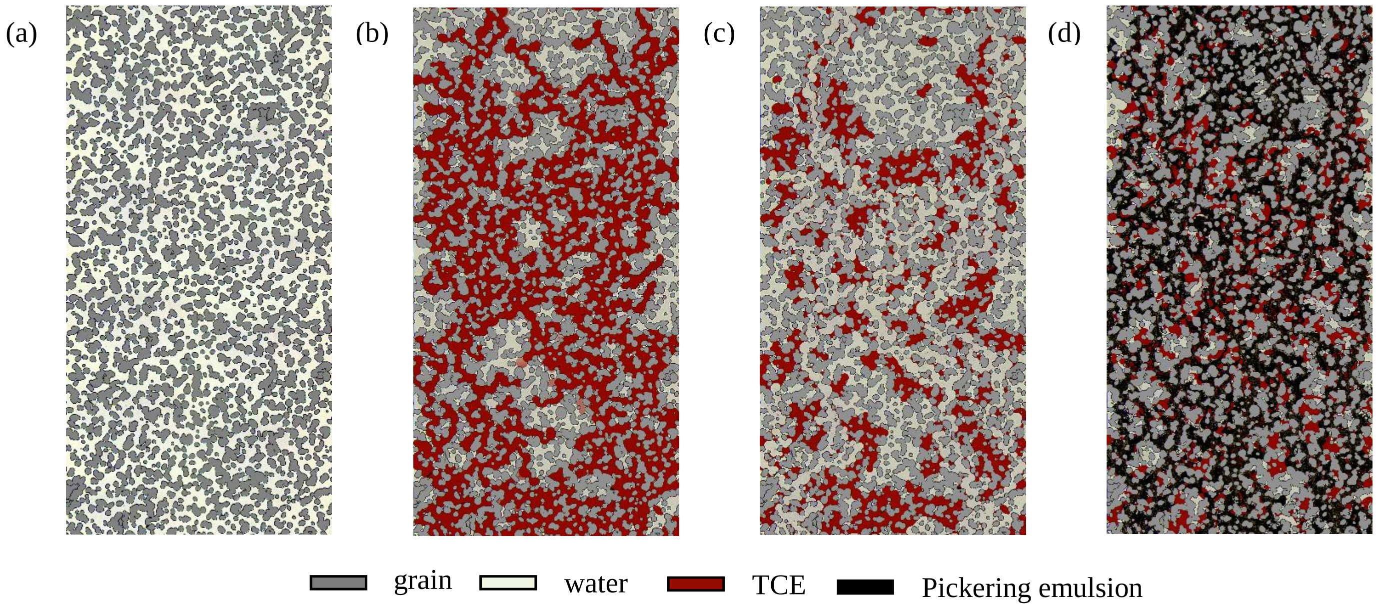

Figure 1. Examples of images at the end of each step of the experiments.

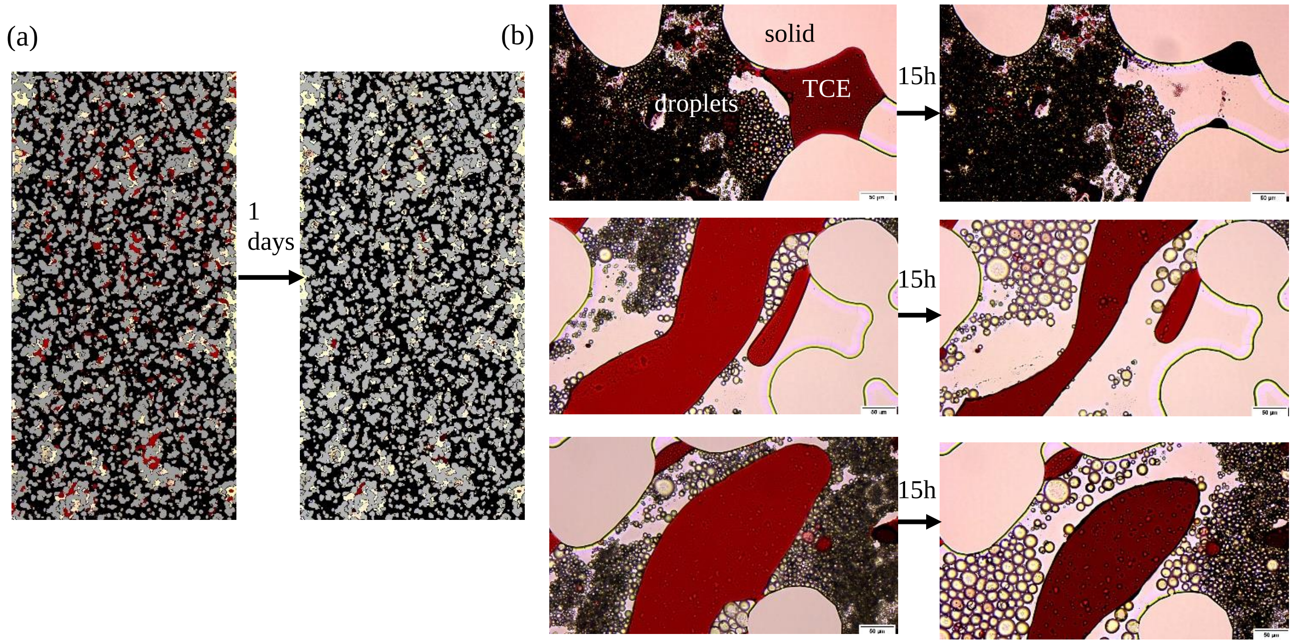

Figure 2. TCE reduction at the static state after emulsion flooding in the whole chip (a) and local area of chip (b).

References

1. van Hullebusch, E. D., Huguenot, D., Pechaud, Y., Simonnot, M. O., & Colombano, S. (2020). Environmental soil remediation and rehabilitation. Springer International Publishing.
2. Chen, Z., Chen, Z., Li, Y., Zhang, R., Liu, Y., Hui, A., Cao, W., Liu, J., Bai, H., & Song, J. (2023). A review on remediation of chlorinated organic contaminants in soils by thermal desorption. Journal of Industrial and Engineering Chemistry.
3. Sweeny, K. H. (1980). U.S. Patent No. 4,219,419. Washington, DC: U.S. Patent and Trademark Office.
4. Stefaniuk, M., Oleszczuk, P., & Ok, Y. S. (2016). Review on nano zerovalent iron (nZVI): from synthesis to environmental applications. Chemical Engineering Journal, 287, 618-632.
5. Jia, H., He, J., Xu, Y., Wang, T., Zhang, L., Fan, F., Qin, X., Li, Z., Lv, K., & Wang, Y. (2021). Synthesis of hybrid dendritic mesoporous silica titanium nanoparticles to stabilize Pickering emulsions for enhanced oil recovery. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 628, 127237.

Experimental study of the impact of groundwater level fluctuations on the mobilization of petroleum hydrocarbons - geophysical strategy

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Keywords: groundwater level fluctuations, mobilization, *petroleum hydrocarbons.*

NAPLs are immiscible organic contaminants poorly soluble in water, moving through soils and groundwater as oily liquids (Bin Lu et al, 2017). This work focuses on LNAPLs, lighter than water and primarily consisting of refined petroleum hydrocarbons, a common type of worldwide pollutant. LNAPL recovery methods include pumping/skimming, slurping and passive techniques like recovery trench. However, residual LNAPL remains trapped as ganglia or blobs influenced by environmental characteristics and fractionation processes. The remobilization of this residual pollution depends on groundwater fluctuations and the rheological properties of pollutants, varying with environmental heterogeneity and contamination nature (Cavelan A. et al, 2024). Geophysical imaging, especially complex electrical resistivity or induced polarization (IP) offers a non-intrusive and continuous solution to fill information gaps regarding hydrocarbon pollution (Colombano S. et al, 2021; Iravani M. A. et al, 2022). During groundwater fluctuations, LNAPL undergoes changes in distribution and chemical nature (pure, dissolved, and gaseous phases), requiring precise geochemical characterization to calibrate geophysical responses.

In this work, we propose to present the developed geophysical strategy (combining multiphase modelling with complex electrical resistivity) in a multiphase environment typical of an LNAPL-contaminated aquifer, linking responses to organic contaminant characteristics. This combined approach will improve the interpretation of geophysical measurements in the laboratory, on large-scale lysimeter setups (Fig. 1) under controlled conditions, and at a polluted field site. Therefore, experimentation, numerical resolution of transport equations, and calibration of geophysical signals through fine molecular analysis of contaminants in various compartments (pure, dissolved, gaseous phases) will allow for assessing pollutant variations induced by groundwater fluctuations.

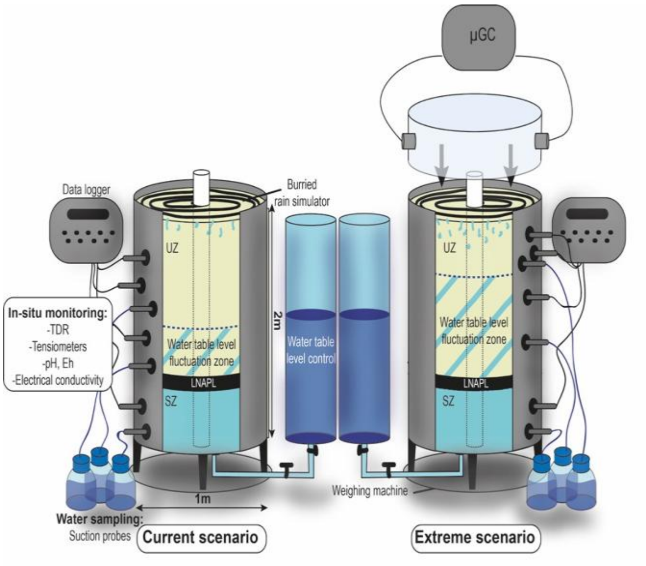

Fig. 1. Instrumented lysimetric column.

This work is included in the GISFI scientific research consortium (http://www.gisfi.univ-lorraine.fr).

References

1. Bin Lu, Shiqiang Wu, Xinghua Xie, and Yefei Tan; The behaviors of LNAPL migration and entrapment in a rough-walled vertical fracture; Geosciences Journal; Volume 21; 407-416 (2017).
2. Amélie Cavelan, Pierre Faure-Catteloin, Catherine Lorgeoux, Stéfan Colombano, Jacques Deparis, Dorian Davarzani, Noële Enjelvin, Constantin Oltean, Anne-Julie Tinet, Fabien Domptail, Fabrice Golfier; An experimental multi-method approach to better characterize the LNAPL fate in soil under fluctuating groundwater levels; Journal of Contaminant Hydrology; Volume 262; (2024).
3. Mohammad Ali Iravani, Hossein Davarzani, Jacques Deparis, Stéfan Colombano, Nicolas Philippe, Benjarese Oniangue, Roger Guérin, Alexis Maineult; Experimental study of electrical complex resistivity in a 2D multiphase porous medium under non-isothermal conditions: Application to soil remediation monitoring ; Near Surface Geophysics, Volume 21 ; 65-81 (2022).
4. S. Colombano, H. Davarzani, E.D. van Hullebusch, D. Huguenot, D. Guyonnet, J. Deparis, I. Ignatiadis; Permittivity and electrical resistivity measurements and estimations during the recovery of DNAPL in saturated porous media: 2D tank experiments; Journal of Applied Geophysics; Volume 191, (2021).

Drying Dynamics in Biological Materials Revealed by NMR: Potatoes as a Case Study

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Keywords: Drying, Biological porous media, NMR

The drying of biological materials, such as vegetables and fruits, is crucial for enhancing shelf life, maintaining nutritional value, and reducing transportation costs. Potatoes, an essential global carbohydrate source, illustrate the complexity of drying biological tissues due to their cellular structure and the coexistence of multiple water states: intercellular free water, cell-wall-associated water, and strongly bound water adsorbed onto starch. Each type of water has distinct transport mechanisms, complicating accurate modelling and optimization of the drying process. In this study, Nuclear Magnetic Resonance (NMR) techniques are used to explore potato drying dynamics, precisely identifying the different water populations based on their T_2 relaxation times [1]. One-dimensional drying experiments were conducted on cylindrical potato samples under varying dry air flux conditions. Under low-intensity airflow, a clear constant-rate drying period was observed, corresponding first to the extraction of free water, then cell wall water, followed by a declining rate associated exclusively with bound water removal. Under high-intensity airflow, drying rate declined continuously from the beginning, with simultaneous extraction of free water from intercellular spaces and cell walls, and subsequent removal of bound water. Additionally, significant shrinkage occurred during initial drying, associated primarily with free water extraction and cellular collapse. As drying progressed, shrinkage ceased, leading to void pores between compacted starch granules, shifting moisture transport from liquid-phase to bound water-vapor diffusion. These structural evolutions are illustrated schematically in Figure 1, clarifying the complex coupling between water states and structural changes. Based on our experimental observations, we developed a simple diffusion model integrating shrinkage effects and distinct drying regimes. The model effectively distinguishes diffusion coefficients for main drying stages, offering a practical framework to optimize drying parameters, reduce energy usage, and enhance the quality of dried potato products.

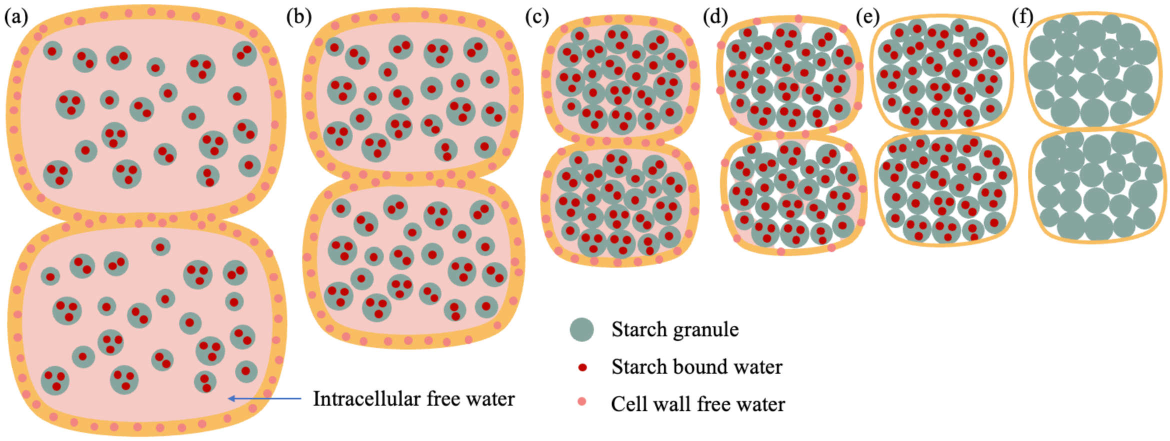

Fig 1. Schematic representation of structural changes during potato drying: (a) Initial saturated state, (b) Onset of shrinkage due to free water extraction, (c) End of shrinkage with maximum cellular collapse, (d) Unsaturated drying with stable volume and emerging pores, (e) State with complete removal of free water, and (f) Final dried state showing interconnected pores facilitating vapor transport.

References

[1] Maillet et al. Dynamic NMR relaxometry as a simple tool for measuring liquid transfers and characterizing surface and structure evolution in porous media. *Langmuir*, 38 (49), 15009-15025 (2022)

Characterization of Drag and Permeability of Dendritic Grains by Numerical Simulations

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Keywords: drag, permeability, dendrite, solidification, lattice Boltzmann method

During the solidification of metallic alloys, the solid grows in form of dendritic grains. The transport of these grains in the liquid significantly influences the structure and chemical segregation in the final product. Capturing the coupling of grain motion with fluid flow is crucial for solidification process simulations. Because grains in the µm range cannot be fully represented in process-scale simulations, constitutive laws are necessary to describe the forces acting on them. We perform direct simulations of Stokes flow around dendrites and we determine specific constitutive laws for drag and permeability that account for the complex shape of dendritic grains and can be used in simulations where their geometry is not fully described.

We simulated the flow around different dendrites, obtained from phase field simulations of solidification [1], as static immersed boundaries in lattice Boltzmann simulations [2]. We processed the force, velocity, and pressure fields to derive drag laws that can be used in simulations modelling grains as point particles. Furthermore, we determined permeability fields that can be used in grain envelope models [3] that describe dendrites as permeable particles.

We propose a drag correction factor for dendrites expressed as a function of the their morphology and of the confinement of the dendrite in a periodic array, ranging from dilute to packed. A description of dendrites as porous *dendrite envelopes* – permeable particles with a shape that envelops the tips of the dendrite branches – is also investigated. Using a permeability field together with a volume-average description of the flow through the dendrite envelope can be used to determine the distribution of the forces acting on the fluid and on the dendrite. We propose new constitutive relations for the permeability of dendrite envelopes.

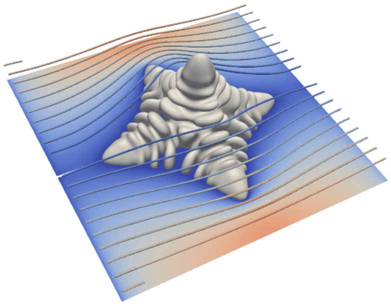

Figure 1: Velocity field (zero in blue to maximum magnitude in red) around a dendritic grain.

References

[1] D. Tourret, L. Sturz, A. Viardin, M. Založnik, Comparing mesoscopic models for dendritic growth, *IOP Conf. Ser.: Mater. Sci. Eng.* 861, 012002 (2020).

[2] J. G. M. Eggels, J. A. Somers, Numerical simulation of free convective flow using the lattice-Boltzmann scheme, *Int. J. Heat Fluid Flow*, 16, 357–364 (1995).

[3] A. Olmedilla, M. Založnik, H. Combeau, Quantitative 3D mesoscopic modeling of grain interactions during equiaxed dendritic solidification in a thin sample, *Acta Mater.* 173, 249–261 (2019).

Foam coarsening dynamics within non-Newtonian fluids

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Keywords: Foam coarsening, Non-Newtonian, Gas diffusion, Cellulose nanofibrils

Injecting additive-stabilized foam fluids presents a promising approach for geological carbon storage (GCS) in complex reservoir environments. The effectiveness of this technique critically depends on foam stability and flow behaviour within a confined space. However, the mechanisms governing the transition from foam coarsening to structural equilibrium, especially in non-Newtonian systems, remain insufficiently understood. This study investigates the gas-diffusion-driven coarsening of quasi-2D foams in non-Newtonian fluids, and the interaction between fluid rheology and gas diffusion in shaping foam morphology. Non-Newtonian precursor fluids were prepared using cellulose nanofibrils (CNF), and their rheological properties were systematically correlated with foam evolution. Fluorescence imaging combined with custom analysis tools enabled quantitative tracking of bubble morphology and dynamics. Results show that increasing CNF concentration leads to a nonlinear enhancement in foam stability, as indicated by extended half-life times. Analysis of bubble size distribution and lamella curvature revealed that higher CNF content suppresses gas diffusion and bubble rearrangement, especially within confined pore spaces. Overall, this work reveals how non-Newtonian rheology modulates foam stability and structure, offering valuable insights into the design of more effective foam-based GCS strategies under challenging reservoir conditions.

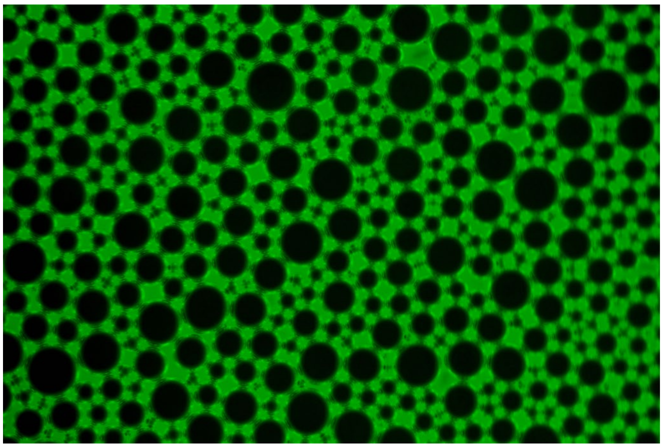

Figure 1: Morphology of CNF-stabilised bubbles under fluorescent microscope.

Use Of Functionalized mesoporous Carbons In Production of ^{165}Er

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Keywords: Radiolanthanides, Separation, Porous carbon

Radionuclides emitting Auger electrons are of interest in Targeted Radionuclide Therapy (TRT) (cancer diagnosis, preclinical studies, radiolabeling, imaging) [1]. Among them, ^{165}Er (T = 10.36 h) is a pure Auger Electron (AE) emitter and a useful tool for fundamental studies on the biological effects of AE emitter. Irradiations of natural holmium target is an easy access to ^{165}Er production :

- directly using proton or deuteron beam : most usual form of radionuclide production
- undirectly via ^{165}Tm ($T_{½}$ = 30.06 h) which decreases to ^{165}Er : concept of generator.

In all cases, separation of lanthanides is challenging, moreover with adjacent lanthanides as the pair Ho/Er or Er/Tm. They have similar oxidation states, coordination chemistry, or unfavorable mass ratio in the target (e.g., 1:10^4 for ^{165}Er:Ho) [2]. Radiochemical separations of lanthanides may be performed by solid−liquid extraction methods using functionalized porous supports. In this regard, recent works have highlighted potential advantages of porous carbons as support over other due to their higher stability under harsh irradiation conditions, easy functionalization, low cost and versatile of forms and pore architectures [3].

The objective of this study was the use of functionalized mesoporous carbons (various types and physicochemical specifications) in the radiochemical separation of lanthanides in the production of 165Er. Two different process of production were studied: 1) direct production (Ho → Er, 2) generator 165Tm/165Er.

For application 1), the carbons were impregnated with acidic organophosphorous extractant and other derivatives (via physical adsorption) commonly used in commercial resin to separate lanthanides (4). Extractive performance in static (coefficient of distribution (Dw)) and dynamic tests have demonstrated similar profile of separation of ^{165}Er/Ho using lower concentration of nitric acid compare to equivalent commercial LN resin. Such improved extraction performance (obtained with named CV porous sample) for the recovery is explained by the tight immobilization of the ligand inside the pores, thereby increasing the stability. For application 2), CV porous carbon was functionalized with DOTA molecule to be used as a support of generator ^{165}Tm/^{165}Er. First results demonstrated no separation between ^{165}Tm and ^{165}Er complexed in form of [^{165}Tm]Tm-DOTA or [^{165}Er]Er-DOTA. No traces of free ^{165}Er eluted from the generator ^{165}Tm/^{165}Er.

References

[1] A Ku and coll. Auger electrons for cancer therapy – a review, *EJNMMI Radiopharm Chem Journal*, 4, 27 (2019).
[2] I. Da Silva and coll. A high separation factor for165 Er from ho for targeted radionuclide therapy, *Molecules*, 26-(24), 7513 (2021).
[3] L. Lefrançois Perreault and coll., Functionalization of Mesoporous Carbon Materials for Selective Separation of Lanthanides under Acidic Conditions *ACS Appl. Mater. Interfaces* 9, 12003 (2017),
[4] D. R. McAlister and coll. Characterization of Extraction of Chromatographic Materials Containing Bis(2-ethyl-1-hexyl)Phosphoric Acid, 2-Ethyl-1-Hexyl (2-Ethyl-1-Hexyl) Phosphonic Acid, and Bis(2,4,4-Trimethyl-1-Pentyl)Phosphinic Acid, *Solvent Extr. Ion Exch.*, 25-(6), 757–769, (2007)

Multi-Scale Heterogeneities in a Complex Limestone Formation: Imagery and Petrophysical Characterization

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Keywords: porous heterogeneities, structure imagery, upscaling

The structure of the heterogeneities of hydrogeosystems such as pores, cracks, fractures, karstic networks controls the fluid and heat transfers, water quality and its availability. Complex systems typically include multiple porosities at embedded scales, from the micro/meso cracks and pores to geological macro-fractures and karsts. This complex network plays interdependent roles and introduces difficulties in the characterization of the whole formation dynamics, especially with difficulties extrapolating laboratory interpretation to field investigation.

The characterization at all scales of the structures of the porous heterogeneities is the objective of this study. We aim to define the structural REV (Repsentative Elementary Volume – [1]) and to develop scale laws capturing the evolution of these networks, considering micrometric to metric heterogeneities. It implies the use of different methods to characterize the medium and sensors at various frequencies to deal with the upscaling. The idea is to face (when possible) direct imagery to indirect acoustic imagery at three scales: (i) micro to centimetric heterogeneities considering thin sections to small cores, using direct imagery and micro-tomography ; (ii) decimetric heterogeneities using both direct imagery and indirect acoustic imagery ; (iii) metric to larger heterogeneities considering outcrop 3D scan and field seismic survey.

Our study focusses on the platform “Observatoire des transferts dans la Zone Non-Saturée” (O-ZNS, Orléans, France), an artificial excavation in the karstified and fractured limestone formation of Beauce aquifer.

The first investigation made on the smallest scale allows us to develop image processing tools. It also highlights the control of heterogeneities on the flow properties and shows the possibilities (and limitations) of acoustic measurement to predict porosity, mainly when facing microporosity [2]. The intermediate scale is still under investigation but already show good correlation between the observed structure and the obtained acoustic and flow signals. Finally, the largest scale of O-ZNS outcrop is under investigation. Larger structures are observed and correctly fit to 3D georadar survey [3].

References

[1] Bear, J. Dynamics of fluids in porous media. *Courier Corporation*. Link (1988)
[2] Yacouba, A.N., Mallet, C., Jougnot, D., Leroy, P., Laurent, G., Beck, K., Gaboreau, S., Azaroual, M. & Deparis, J. (under review). Transport properties estimation from coupled acoustic and electric characterization in heterogeneous limestones. *Jr of Applied Geophysics*. Pre-print on Hal: https://hal.science/hal-04520290. (2025)
[3] Mallet, C., Jodry, C., Isch, A., Laurent, G., Deparis, J. & Azaroual, M.. Multi-geophysical field measurements to characterize a multi-scale karstic and fractured limestone vadose zone: Beauce aquifer. *In Instrumentation and Measurement Technologies for Water Cycle Management.* DOI: 10.1007/978-3-031-08262-7_19 (2022)

Liste des auteurs

Mardi 4 novembre 2025

Session parallèle 1	*Imagerie et caractérisation des milieux poreux I* *Imaging and characterization of porous media I*	
10:15	Imaging solute transport in 3D printed porous media	Lamblin Marc - Géosciences (Rennes France)
10:35	3D visualization of fast two-phase flows in porous media using a laboratory x-ray CT scanner	Oxarango Laurent - Institut des Géosciences de l'Environnement (UGA - IGECS Grenoble, France)
10:55	Morphology probed locally through tortuosimetric analysis	Chaniot Johan - Institut Mines-Télécom (France)
11:15	~~Exploring water transport and aging mechanisms in bio-based porous materials through NMR relaxometry~~	~~Sidi-Boulenouar Rahima - Université Gustave Eiffel (France)~~
11:35	~~Fluid transfers through dynamic NMR relaxometry~~	~~Maillet Benjamin - Navier Laboratory (Champs-sur-Marne, France)~~
Session parallèle 1	*Transport colloïdal et particulaire en milieu poreux* *Colloidal and particle transport in porous media*	
10:15	Pore-scale modelling of diffusiophoresis for groundwater remediation	Cajot Florian - Institut des Sciences de la Terre d'Orléans (France)
10:35	Stochastic modeling and simulation of particle bridging in constricted channels	Maya Fogouang Laurez - Institut des Sciences de la Terre d'Orléans (France)
10:55	Progressive clogging via dendrite growth in porous media	Okaybi Walid - Institut des Sciences de la Terre d'Orléans (ISTO) (France)
11:15	~~Flow induced intermittent transport shapes colloid filtration in porous media~~	~~De Anna Pietro - Université de Lausanne (Suisse)~~
11:35	~~Modeling of the Hydrophobic Treatment of Gas Diffusion Layers to predict PTFE distribution~~	~~Arnelli Pierluigi - Laboratoire d'Innovation pour les Technologies des Energies Nouvelles et les nanomatériaux (France)~~
Session parallèle 1	*Milieux confinés, nano-échelles et modélisation moléculaire* *Confined media, nanoscale and molecular dynamics*	
10:15	Fluctuations enhance diffusive transport in nanopores	Marbach Sophie - PHysicochimie des Electrolytes et Nanosystèmes InterfaciauX (France)
10:35	Insights Into Bangham's Law With Molecular Simulations: Surface Stress vs. Surface Tension in C-S-H	Leng Jingyi - Laboratoire Navier (France)
10:55	Texture-based assessment of gas adsorption selectivity on porous carbons with enhanced separation properties	Schaefer Sébastien - Interfaces, Confinement, Matériaux et Nanostructures (France)
11:15	~~Thermodynamic and structural insights into water intrusion in ZIF-8 using calorimetry and neutron diffraction~~	~~Marescot Thomas - LLB - Matière molle et biophysique (France)~~

Mardi 4 novembre 2025

Session parallèle 2	*Ecoulements multiphasiques en milieux poreux I* *Multiphase flows in porous media I*	
14:30	Influence of wettability on water relative permeabilities curves in unconsolidated porous media: from water-wet to oil-wet	Hernandez Perez Kevin - Institut Terre Environnement Strasbourg (France)
14:50	Disorder-induced non-linear growth of fingers in immiscible two-phase flow in porous media	Meheust Yves - Géosciences Rennes (France)
15:10	Modeling approaches for drainage instabilities in porous media: phase-field versus dynamic capillary pressure modeling	Ommi Siddhartha H. - Institut de Recherche en Génie Civil et Mécanique (GeM) (France)
15:30	Pilot-scale investigation of LNAPL transport under dynamic water table conditions: 3D three-phase flow experiments and simulations	Alamooti Amir - GeoRessources (France)
Session parallèle 2	*Mécanique, poromécanique, rupture, endommagement* *Mechanics, poromechanics, fracture, damage*	
14:30	Friction modifies poroelasticity of a yeast clog	Liot Olivier - Institut de mécanique des fluides de Toulouse (France)
14:50	Micro-mechanical study of hydro-mechanical coupling at the interfaces of raw Earth masonry	Georges David - Laboratoire sols, solides, structures - risques [Grenoble] (France)
15:10	Implementing contact-mechanics in faulted porous media using VEM	Chassonnery Pauline - Bureau de Recherches Géologiques et Minières (BRGM) (France)
15:30	Skin factor model for CO2 injection in coalbed reservoir	Le Tien Dung - Laboratoire d'Energétique et de Mécanique Théorique et Appliquée (Vandoeuvre-lès-Nancy, France)
Session parallèle 2	*Mésoporeux* *Mesoporous*	
14:30	Use of functionalized mesoporous carbons in production of 165Er	Da Silva Isidro - CNRS CEMHTI (Orléans, France)
14:50	NH3-responsive chromism of cyanine dyes adsorbed on surface-modified mesoporous silica	Sohmiya Minoru - Idemitsu Kosan Co.,Ltd. (Japon)
15:10	Quantification of the pore connectivity in mesoporous carbons by analyzing hysteresis scanning curves	Ania Conchi - Conditions Extrêmes et Matériaux : Haute Température et Irradiation (France)

Mardi 4 novembre 2025

Session parallèle 3	*Microfluidique* *Microfluidics*	
16:15	Measurements of concentration gradients in geological porous media using microfluidics devices and Raman spectroscopy	Sarr Mohamadou - Institut des Sciences de la Terre d'Orléans (France)
16:35	Tuning wettability of microfluidics via in situ plasma treatment	Douat Claire - Groupe de recherches sur l'énergétique des milieux ionisés (France)
16:55	Crystallization of sodium chloride in microfluidic pore systems	Genetelli Jade - Laboratoire d'Analyse et d'Architecture des Systèmes - Equipe MILE (France)
17:15	Pore-scale study of pickering emulsions for chlorinated solvent remediation via compositional ripening	Wang Shuxin - Arts et Metiers Institute of TechnologyA (France)
Session parallèle 3	*Transfert thermique en milieux poreux* *Heat transfer in porous media*	
16:15	Selection of convection cells during convective instabilities in heterogeneous porous media: state of the art benchmarking	Quintin Elliot - IFP Energies nouvelles (France)
16:35	Coupled heat and moisture transfer in porous building materials: accounting for the sorption hysteresis	Benmahiddine Ferhat - École Spéciale des Travaux Publics, du Bâtiment et de l'Industrie [Paris] (France)
16:55	Simulation of a porous iron particle melting in a fluid	Robin Jean - Institut Jean Le Rond d'Alembert (France)
17:15	Improved modelling of the conduction-radiation coupling in heterogeneous media by a fully stochastic approach	Roch Mattéo - CEA Le Ripault (France)
Session parallèle 3	*Transferts en milieux fracturés* *Transfers in fractured media*	
16:15	The dual porosity approach for modelling seawater intrusion in fractured aquifers	Koohbor Behshad - GeoRessources (France)
16:35	Analysis of heat transport in fracture networks with dead ends	Ringel Lisa Maria - Géosciences Rennes (France)
16:55	Capturing multi-scale fracture effects in CO2 storage modelling under uncertainty	Perez Sarah - Heriot-Watt University (Edinburgh, Royaume-Uni)
17:15	An efficient approach to model fluid flow and heat transfer in fractured rock: application in geothermal energy	Alawieh Nour - GeoRessources (France)

Mercredi 5 novembre 2025

Session parallèle 4	*Imagerie et caractérisation des milieux poreux II* *Imaging and characterization of porous media II*	
09:30	Evolution of cohesive contact surface area in biocemented granular meda characterized by X-ray microtomography	Naillon Antoine - Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, Grenoble, France
09:50	Direct experimental quantification of salt-induced permeability reduction in porous media	Ben Elhadj Hamida Syrine - Universite de Pau et des Pays de l'Adour, CNRS, LFCR,DMEX, Pau, France
10:10	Characterization of Porous Metallic Structures Made by Additive Manufacturing for Heat Pipe Applications	Kodio Vincent - LABORATOIRE DE MODÉLISATION ET MATÉRIAUX POUR LA MÉTALLURGIE (France)
Session parallèle 4	*Transport réactif I* *Reactive transport I*	
09:30	Multiscale reactive transport modeling of ion transport in charged porous media	Tournassat Christophe - Earth Science Division [LBNL Berkeley] (États-Unis) - Institut des Sciences de la Terre d'Orléans (France)
09:50	Clayrock electrokinetic coupling modelling using Lattice Boltzmann Method	Tinet Anne-Julie - Laboratoire GeoRessources (France)
10:10	Water flow and solute transport in low-cost porous adsorbents: application to olive mill waste water filtration	Lamy Edvina - Université de Technologie de Compiègne (France)
Session parallèle 4	*Méthodes numériques* *Numerical methods*	
09:30	Development of a new-well balanced numerical scheme for compressible porous media flows	El Ouafa Simon - Université Paris-Saclay, UVSQ, CNRS, CEA, Maison de la Simulation, Gif-sur-Yvette, France (France)
09:50	Enhancements in large-scale hydraulic flow modeling	Parisot Martin -Inria Université de Bordeaux
10:10	Eliminating contact angle in pore-scale two-phase flow: an OpenFOAM-based approach	Norouzisadeh Mojtaba - Institut des Sciences de la Terre d'Orléans (France)

Mercredi 5 novembre 2025

Session parallèle 5	*Imagerie et caractérisation des milieux poreux III* *Imaging and characterization of porous media III*	
11:00	Pore size distribution of Lorrain coal using NMR relaxometry and cryoporometry	Jiang Minchuan - Laboratoire Energies et Mécanique Théorique et Appliquée (France)
11:20	Impact of sedimentary and diagenetic heterogeneities on petrophysical properties (porosity, permeability, P wave velocity) of continental limestones	Jamey Thibaut - Institut des Sciences de la Terre d'Orléans (France)
11:40	Optical thermometry for dynamic imaging of heat transport in analog porous media	Rashed Arwa - Univ. Rennes, CNRS, Géosciences Rennes (France)
12:00	Free and bound water transport during drying of clay material as observed by NMR	Ait Chekh Yousra - Laboratoire Navier (France)
Session parallèle 5	*Milieux poreux biologiques I* *Biological porous media I*	
11:00	Spatio-temporal characteristics of a proliferating saccharomyces cerevisiae clog	Ghenni Mathieu - Institut de mécanique des fluides de Toulouse (France)
11:20	Bioclogging and its impact on biodegradation in NAPL-contaminated sites	Eddaoui Noura - Institut des Sciences de la Terre d'Orléans (France)
11:40	Drying dynamics in biological materials revealed by NMR: potatoes as a case study	Zou Yuliang - Laboratoire Navier (France)
12:00	Water transfer in starch-fibers composite	Hbaieb Olfa - Laboratoire Navier (France)
Session parallèle 5	*Ecoulements multiphasiques en milieux poreux II* *Multiphase flows in porous media II*	
11:00	Determination of the relative permeability of earthen material during drying using Magnetic Resonance Imaging	Keita Emmanuel - Laboratoire Navier (Champs-sur-Marne France)
11:20	Impact of inertia on the stability of two-phase flow: a pore-doublet approach	Bernard Nathan - Institut des Sciences de la Terre d'Orléans (France)
11:40	Thin film flow: fluid transport via thin liquid film in slow porous media flows	Moura Marcel - PoreLab - University of Oslo (Norvège)
12:00	Enhancements in large-scale subsurface flow modelling	Erdocio Sebastien - IFP Energies nouvelles (France)

Mercredi 5 novembre 2025

Session parallèle 6	*Modèles numériques et couplage pour les milieux poreux* *Numerical models and couplings for porous media*	
15:15	Field scale Thermo-poro-mechanical modelling for CO2 storage	Bourgeois Frederic - Centre scientifique et Technique Jean Feger (France)
15:35	Modeling complex flows in porous media with ComPASS	Smai Farid - BRGM (Orléans France)
15:55	A THMC approach for crack appearance within reactive porous media under hydrochemo-mechanical loads	Seigneur Nicolas - Mines Paris PSL (France)
16:15	Coupled thermo-hydro-mechanical uncertainties for CO2 storage integrity assessment	Pillardou Nicolas - CHLOE - UPPA (France)
Session parallèle 6	*Transport, mélange et dispersion en milieu poreux* *Transport, mixing and dispersion in porous media*	
15:15	Dispersion in porous media: A comprehensive numerical comparison of existing methods	Grigorov Emil - Aix Marseille Universite, CNRS, IUSTI, Marseille (France)
15:35	Convective dissolution of CO2 in index-matched porous media: a shadowgraphy study	Imuetinyan Happiness - Laboratoire des Fluides Complexes et leurs Réservoirs (France)
15:55	Incomplet mixing in chaotic flows	Heyman Joris - - Géosciences Rennes (France)
16:15	Intrinsic permeability of heterogeneous porous media	Jiao Wenqiao - University of Lausanne / Institute of Earth Sciences (Suisse)
Session parallèle 6	*Fluides complexes, non-newtoniens, inertiels et turbulents* *Complex, non-Newtonian, inertial and turbulent fluids*	
15:15	Numerical simulations of turbulent flows in double porosity media	Roncen Remi - ONERA, Université de Toulouse (France)
15:35	Characterization of Drag and Permeability of Dendritic Grains by Numerical Simulations	Založnik Miha - Institut Jean Lamour (France)
15:55	Poiseuille flow for S-shaped shear-thickening fluids: streamwise banding and viscous sandglasses	Talon Laurent - Fluides, automatique, systèmes thermiques (ORSAY, France)
16:15	~~Foam coarsening dynamics within non-Newtonian fluids~~	~~Zhou Tongke - China University of Petroleum Beijing (Chine)~~

Jeudi 6 novembre 2025

Session parallèle 7	*Imagerie et caractérisation des milieux poreux IV* *Imaging and characterization of porous media IV*	
09:30	19F magnetic resonance imaging-informed of PFAS in porous media	Peyneau Pierre-Emmanuel - Eau et Environnement (France)
09:50	Evaporation of a sodium chloride aqueous solution from a porous medium: dome efflorescence formation	Oumeima Souissi - Laboratoire Matériaux et Durabilité des constructions (France)
10:10	Impact of Saturation Level and Water Redistribution on Carbon Mineralization in Unsaturated Porous Media	Golmohammadi Meysam - Institut des Sciences de la Terre d'Orléans (France)
Session parallèle 7	*Couplages multiphysiques en milieux poreux I* *Multiphysics couplings in porous media I*	
09:30	Water retention curve of PEM fuel cell catalyst layer from numerical simulations on 3D digital images	Flaumenbaum Paul - Institut de mécanique des fluides de Toulouse (France)
09:50	Gas transport through porous media induced by a temperature gradient	Graur Irina - IUSTI (Marseille France)
10:10	Theory and lattice Boltzmann modeling of pollutants in solution: effect of the porous medium heterogeneity on adsorption and transport	Ben Amor Nada - Laboratoire Interdisciplinaire de Physique (Saint Martin d'Hères, France)
Session parallèle 7	*Milieux fibreux* *Fibrous media*	
09:30	Benchmark exercise on the numerical prediction of permeability of anisotropic fibrous materials	Syerko Elena - Nantes Université, Ecole Centrale Nantes, CNRS, GeM (France)
09:50	Free surface flow around and inside an amphiphilic porous hollow fiber	Beltrame Philippe - Environnement Méditerranéen et Modélisation des Agro-Hydrosystèmes (France)
10:10	Radiative characterization of a fibrous medium by cylinder stack morphological study and Monte Carlo method	Souveton Mahé - Thermique aux Nano échelles et Rayonnement [Institut Pprime] (France)

Jeudi 6 novembre 2025

Session parallèle 8	*Transport réactif II* *Reactive transport II*	
11:30	Machine learning for geochemistry and application to thermal reactive transport	Michel Anthony - IFP Energies nouvelles (France)
11:50	Hydro-Mechano-Chemical Coupling for the Simulation of Pore-Scale Integrity in Crystallization Process	Poncet Philippe - Laboratoire de Mathématiques et de leurs Applications [Pau] (France)
12:10	~~Numerical study of reactive transport in unsaturated porous media~~	~~Wang Hui - Géosciences Rennes (France)~~
Session parallèle 8	*Couplages multiphysiques en milieux poreux II* *Multiphysics couplings in porous media II*	
11:30	Multi-physics simulation of void evolution in thermoset prepreg UD laminates	Briard Anne-Lise - Institut Clément Ader (France)
11:50	Refined porous ceramic manufacturing using active learning	Gopale Gowda Jnanesh - École des Mines de Saint-Étienne (France)
12:10	A physical approach to the modeling of hygrothermal transfers in bio-based building materials	Daunais Nicolas - Laboratoire Navier (France)
Session parallèle 8	*Ecoulements multiphasiques en milieux poreux III* *Multiphase flows in porous media III*	
11:30	Modeling and simulation of ocean-groundwater interactions through the beach: a Navier-Stokes and Richards equations coupling	Bonnet Tony - Institut de Mécanique et d'Ingénierie (France)
11:50	Advantages of physics neural networks for modeling seawater intrusion in coastal aquifers	Mansouri Bajgiran Maryam - Institut Terre Environnement Strasbourg (France)
12:10	~~Modeling groundwater flow in unconfined aquifers with physics-informed neural networks: inverse modeling~~	~~Asghari Meinagh Parisa - Institut Terre Environnement Strasbourg (France)~~

Jeudi 6 novembre 2025

Session parallèle 9	*Transport réactif III* *Reactive transport III*	
14:45	Reactive percolation in ultramafic rocks: impacts of permeability and pore structure on hydrogen generation	Obin Thomas - Institut des Sciences de la Terre d'Orléans (France)
15:05	Controls of double-porosity interconnectivity on dissolution of carbonate rocks	Briolet Théo - Laboratoire de géologie de l'ENS (France)
15:25	Experimental investigation of salt precipitation in rock samples for hydrogen storage applications	Kalyoncu Gülce - PProGRess/UGCT, Department of Geology, Ghent University (Belgique)
15:45	Scallop formation due to dissolution-driven convection	Hurtis Radoslav - Department of Applied Mathematics and Statistics, Comenius University, Bratislava, Slovakia
Session parallèle 9	*Milieux poreux biologiques II* *Biological porous media II*	
14:45	Porous media modeling of macromolecule diffusivity in the intracellular volume	Chabanon Morgan - Laboratoire d'Énergétique Moléculaire et Macroscopique, Combustion (France)
15:05	Multi-scale characterisation of the porosity in pretreated lignocellulosic biomass	Goc Firat - IFP Energies nouvelles (France)
15:25	Mesofauna activity and soil pore space dynamics: temporal analysis using x-ray microtomography	Cazaurang Simon - Environnement Méditerranéen et Modélisation des Agro-Hydrosystèmes (France)
Session parallèle 9	*Couplages multiphysiques en milieux poreux III* *Multiphysics couplings in porous media III*	
14:45	Conduction-radiation coupling: Characterisation of the effective thermal properties of geopolymers	Fortunat Adjovi Alexandra - IMT École nationale supérieure des Mines d'Albi-Carmaux (France)
15:05	Moisture behavior in textiles: a dynamic NMR study	Gerony Floriane - Laboratoire Navier (France)
15:25	Averaging random conduit networks, influence of conductivity randomness	Colecchio Iván - IFP Energies nouvelles (France)
15:45	Dynamic Displacement of Wetting Fluids by Non-Wetting Fluids in Geological Fractures: an Analog Experiment	Yves Meheust - Université de Rennes, CNRS, Géosciences Rennes (France)

Posters

Experimental Study of Tidal Oscillatory Flows on a Partially Saturated 1D Porous Column	Alastal khalil - Institut de mécanique des fluides de Toulouse (IMFT) (France)
Gas Adsorption Characterization of Biochar: Surface Area, Pore Distribution, and Sorption Energy	Amoury Bilal - Microtrac Formulaction SAS (France)
Experimental Characterization of Foam Flow and Gas Trapping in Porous Media	Baigadilov Adil - Bureau de Recherches Géologiques et Minières (France)
Optimizing Surfactant Foam Formulations for Enhanced (Bio)Remediation of Petroleum-Contaminated Soil	Baimaganbetova Sholpan - BRGM, Orléans (France)
Semi-analytical solution for flow with time-varying viscosity in fractured porous media	Belfort Benjamin - Institut Terre Environnement Strasbourg (France)
Assessment of Groundwater Vulnerability to Leachate Contamination Using Hydrodynamic and Geochemical Indicators in Belloua Mountain, Kabylia, Algeria	Benarab Salah - Faculté de technologie, département de génie des procédés de l'environnement, Université de Boumerdès (Algérie)
Experimental Study of Dissolution Patterns resulting from the competition between Forced and Solutal Convection	Berhanu Michael - Laboratoire Matière et Systèmes Complexes (France)
Linking Mineral Reactions with Induced Polarisation: A Microfluidic Study of FeS Formation and Dissolution	Bil Christiaan - Géosciences Rennes (France)
From Anomalous Transport Of Red Blood Cells To O2 Delivery In Vascular Networks	Blons Hugo - Géosciences Rennes (France)
Synthesis and characterization of nickel oxide nanoparticles by the PECHENIN method for Corrosion Protection and Porous Material Reinforcement Applications	Boughrara Saliha - Laboratory of Food Technology Research (LRTA), University of BOUMERDES (Algérie)
A Novel Machine Learning-based Method for Groundwater Modelling involving Aquifer Rainfall Time Response Analysis and Clustering of Groundwater Wells	Breuillard Hugo - Bureau de Recherches Géologiques et Minières (France)
Probing Particle Dynamics Inside Opaque Porous Media Using X-ray Radiography	Carter Adam - PHysicochimie des Electrolytes et Nanosystèmes InterfaciauX (France)
Elastic Properties of Partially Saturated Tournemire Shale at Seismic Frequencies	Chapman Samuel - Laboratoire de Géologie (France)
Euler-Euler Simulations Of Colloidal Transport And Retention At The Pore Scale	Cheikh Nassim - Institut des Sciences de la Terre d'Orléans (France)
Characterization of the porous network and particle density under compression using XCT of a bio-based porous media	Chekai Tinhinane - cerema (France)
Predicting Seismic Response To Fluid Injection Using Machine Learning	Cuvier Arthur - Bureau de Recherches Géologiques et Minières (France)
Assessment of grid resolution for using Poisson-Nernst-Planck equations in reactive transport modeling.	Dackouo Josaphat - BRGM, ISTO (France)
Studying Diffusiophoresis-Driven Colloid Transport in Porous Media Using Microfluidics	Etienne Pauline - Institut des Sciences de la Terre d'Orléans (France)
Simulation Of Reactive Transport Dynamics In Cerebral Microcirculation	Fialkovsky Dimitri - Institut de mécanique des fluides de Toulouse (France)
Water transfers in starch-fibers composites	Hbaieb Olfa - Laboratoire Navier (France)
Mixing in confined heterogeneous porous media	Sajedi Fateme - Université de Lausanne (Suisse)

Posters

Scalable flow modeling in karstic media through graph simplification	Housni Yousra - IFP Energies nouvelles (France)
Dynamics of Gadolinium Oxide Clogging in Porous Media: Insights from 4D X-ray Microtomography	Iqbal Muqeet- - Institut des Sciences de la Terre d'Orléans - UMR7327 (France)
Intrinsic permeability of heterogeneous porous media	Jiao Wenqiao - University of Lausanne / Institute of Earth Sciences (Suisse)
Iterative Coupling Algorithms For Mixed-Dimensionnal Poromechanical Models In Faulted Geological Systems	Jonval Maxime - Inria (France)
Intercooler study using porous media modeling and CFD simulation	Khadidja Boualem - University of Science and Technology of Oran (Algérie)
Streaming Potential Simulation in Variably Saturated Fractured Porous Media	Koohbor Behshad - GeoRessources (France)
Imaging solute transport in 3D printed porous media	Lamblin Marc - Géosciences (Rennes France)
A Versatile Simulator for Multiscale Reactive Transport in Subsurface Environments	Le Trong Emmanuel - Institut des Sciences de la Terre d'Orléans (France)
Direct observation of calcite dissolution with microfluidics and spectral induced polarization. Geochemical and petrophysical modeling	Leroy Philippe – Bureau de Recherches Géologiques et Minières (France)
Multi-Scale Heterogeneities in a Complex Limestone Formation: Imagery and Petrophysical Characterization	Mallet Celine - Institut des Sciences de la Terre d'Orléans (France)
Imaging of solute transport through impermeable inclusions at Darcy scale	Petitjean Clément - Géosciences Rennes (France)
Synthesis and Characterization of Cage-like Mesoporous Silica SBA-16 to Study Cavitation in Confinement	Puibasset Joel - Interfaces, Confinement, Matériaux et Nanostructures (Orléans, France)
Dynamic Displacement of Wetting Fluids by Non-Wetting Fluids in Geological Fractures: an Analog Experiment	Meheust Yves - Géosciences Rennes (France)
Experimental study of the impact of groundwater level fluctuations on the mobilization of petroleum hydrocarbons - geophysical strategy	Wade Alassane - Bureau de recherches géologiques et minières (France)
Flow and phase behavior of nanoconfined aqueous solutions	Boudaoud Abir - Institut Lumière Matière [Villeurbanne] (France)
A Novel Machine Learning-based Method for Groundwater Modelling involving Aquifer Rainfall Time Response Analysis and Clustering of Groundwater Wells	Breuillard Hugo - Bureau de Recherches Géologiques et Minières (France)
Direct observation of calcite dissolution with microfluidics and spectral induced polarization. Geochemical and petrophysical modeling	Leroy Philippe - Bureau de Recherches Géologiques et Minières (France)
Experimental Study of Dissolution Patterns resulting from the competition between Forced and Solutal Convection	Berhanu Michael - Matière et Systèmes Complexes (France)
Smooth Particle Hydrodynamics (SPH) code for fracture and hydrofracture propagation	Dymitrowska Magdalena - Institut de Radioprotection et de Sûreté Nucléaire (France)
Stabilizing Emulsions with Surfactant-Nanomaterial Systems in Carbonated Water Injection for EOR	Khanjani Maral - Nazarbayev University (Kazakhstan)

France InterPore Chapter

17e Journées d'Etudes des Milieux Poreux

Du 4 au 6 novembre 2025 à Orléans

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