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Editorial

Microscopic flow and reactive transport in geological media: Recent advances and challenges

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Abstract:
Microscopic flow and reactive transport in the subsurface are fundamental to understanding the coupled physical, chemical, and biological processes governing subsurface environments. These processes play a critical role in sustainable water resource management, groundwater contamination control and remediation, geological carbon storage, and subsurface energy exploitation. With the escalating impacts of global climate change and anthropogenic activities, interactions among physical and chemical processes in geological media have grown increasingly complex. Consequently, research on flow and reactive transport has emerged as a vibrant and rapidly evolving frontier. A dedicated session entitled "Microscopic Flow and Reactive Transport in Geological Media" was featured at the "2025 International Symposium on Subsurface Reactive Transport" successfully held in Changchun, China, September 19-21, 2025. The symposium served as a platform for interdisciplinary collaboration and knowledge exchange, providing new perspectives and establishing a solid foundation for future scientific cooperation in the field of subsurface reactive transport.

1. Introduction

Microscopic flow and reactive transport in the subsurface involve the coupled transport and transformation of chemical species within geological formations, driven by fluid flow, heat transfer, and geochemical reactions. These processes govern a wide range of phenomena, including contaminant transport and phase partitioning, playing a critical role in the evolution of groundwater systems and subsurface energy reservoirs. As such, they present not only a fundamental mechanism in shaping geological environments but also a fundamental scientific challenge that interlinks biogeochemistry, hydrodynamics, and thermodynamics across multiple spatial and temporal scales.

The coupling among physical, chemical, and biological processes in the subsurface has become increasingly complex as human activities introduce non-native fluids and chemicals. To advance a fundamental understanding of these multiscale interactions is therefore essential for developing predictive models that support the safe and efficient utilization of sub-

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surface resources.

To promote international collaboration and disseminate cutting-edge research in this field, the "2025 International Symposium on Subsurface Reactive Transport" was established as an open and high-level academic platform. The symposium aimed to integrate theoretical advances, laboratory observations, and field applications to address emerging challenges in subsurface flow and reactive transport.

The symposium featured nine thematic sessions. Among them, the session entitled "Microscopic Flow and Reactive Transport in Geological Media" served as a key forum, showcasing recent advances in multiscale coupling, pore-scale visualization, and digital rock simulations, advances that are reshaping our understanding of subsurface flow and reactive transport mechanisms. This editorial provides a brief summary of the insights gained from this session, with the goal of sharing these outcomes with the broader research community.

2. Pore-scale mechanisms of CO_2 storage and multiphase flow

Yongfei Yang, from China University of Petroleum (East China), presented recent advances in pore-scale experiments and simulations focused on CO_2 trapping mechanisms. An integrated experimental platform combining "core-flooding + *in-situ* CT scanning" was developed (Li et al., 2023), which accurately analyzes the distribution characteristics of fluids in pore space and the dynamic changes of pore structure. The system reveals the capillary trapping mechanisms and rock dissolution patterns. A pore-scale flow simulation method based on digital rock has been established, overcoming the limitations of traditional simulation and achieving accurate simulation of multiphase flow in porous media. This provides an efficient and reliable numerical tool for exploration of fluid flow mechanisms. The digital rock experiment technology and nano/micro-scale flow simulation tools have provided key support for the theoretical and applied research of carbon capture, utilization, and storage engineering (Wang et al., 2025a).

Huixing Zhu, from Jilin University, delivered a lecture about a pore-scale numerical method to quantify CO_2 capillary breakthrough pressure across diverse rocks. This work presents a novel lattice Boltzmann method for the direct simulation of multiphase flow in complex three-dimensional porous media, enabling the determination of CO_2 capillary breakthrough pressures across various lithologies (Yang et al., 2025). The results show that although breakthrough pressure is inversely correlated with porosity and permeability, these conventional parameters have limited predictive power. Validation across sandstone, mudstone, and shale confirms the method's broad applicability, offering a fast and reliable approach to predict CO_2 breakthrough pressure in CO_2 geological storage projects.

3. Coupled reactive transport and mineral evolution

Heng Li, from the Eastern Institute of Technology (Ningbo), presented a new multiscale reactive transport model that tackles key limitations of multi-mineral systems. Using the upscaling technique based on the homogenization method, the model of the multi-scale coupled reactive transport can be derived from the pore-scale model. However, the current model still has obvious shortcomings in dealing with the geochemical reactions of multi-mineral systems (Garttner et al., 2022). In order to solve this problem, the model was coupled with existing and widely validated geochemical models, so that it has the ability to handle multi-mineral reactions under complex hydrochemical conditions (Li et al., 2024). The new model manages well the challenging geometrical configurations of multiple interfaces introduced by multiple minerals during the simulation. At the same time, the new model accurately captures the abrupt change of macroscopic effective parameters caused by the change of pore geometries.

Hang Deng, from Peking University, gave a presentation on pore-scale reactive transport modeling of mineral precipitation. Accurate assessment of the evolution of porous media requires predictive understanding of pore-scale reactive transport processes that involve mineral precipitation. The presentation demonstrated the application of micro-continuum reactive transport model as a valuable tool for this purpose. It has been used to successfully simulate nucleation and crystal growth in mixing-dominated systems, and predicted precipitation patterns that are consistent with experimental observations, along with the evolution of effective diffusivity (Deng et al., 2021). The model has also been applied to investigate interface coupled dissolution and precipitation (Deng et al., 2022), and the potential passivation effect on the dissolution of the parent mineral (ongoing work). These pore-scale studies provide valuable insights needed for upscaling important microscopic processes in macroscopic modeling efforts.

Qian Zhang, from the Institute of Geology and Geophysics, discussed how microstructural heterogeneity governs geochemical alteration in fractured rocks. The talk highlighted how geochemically driven alterations in multi-mineral fractured rocks generate altered layers along fracture–matrix interfaces. Enabled by co-designed experiments and micro-continuum simulations, the respective contribution of structural and mineralogical features in fracture–matrix evolution was systematically assessed. The results demonstrated that incorporating spatial heterogeneity in mineral distribution leads to channelized altered layer structures, reduced overall reaction rates, but enhanced permeability. The study further pointed out that coupling between chemical and mechanical processes could complicate altered layer development and potentially trigger matrix disaggregation, erosion, and other alteration mechanisms in fractured systems.

4. Particle transport, clogging and biofilm dynamics

Zhibing Yang, from Wuhan University, presented experimental findings on particle transport and clogging under multiphase flow conditions. Techniques capable of visualizing fluid-fluid displacement and particle transport were introduced and applied to different types of flow cells. Particle behaviors including sedimentation, suspension, deposition and clogging during multiphase displacement were analyzed in detail with comparison to theoretical predictions. The combined effects of hydrodynamic condition and suspension composition on the transition of clogging regimes were elucidated (Zhang et al., 2023). It was discovered that fluid fragmentation and redistribution of the wetting phase can be induced by spontaneous particle aggregation (Wu et al., 2025). The findings emphasized the dynamic coupling between pore-scale particle behaviors and hydraulic and transport properties at larger scales, providing insights for predicting and controlling particle mediated processes in relevant engineering applications.

Xiaofan Yang, from Beijing Normal University, introduced a coupled modeling framework spanning pore- to Darcy-scales. Biofilm formation involves three stages: attachment & aggregation, growth & accumulation, and disaggregation & detachment. A modeling framework was established using a unified set of equations to simulate biofilm processes across both pore and Darcy scales (Li and Yang, 2025). The in-house developed BioFOAM solver incorporates mechanisms such as flow and solute transport, biomass evolution, and fracture-matrix interactions. The study focused on how fracture-matrix flow interactions influence biofilm growth under varying matrix permeabilities and initial biomass attachment sites. Results showed that higher matrix permeability enhances biofilm growth by promoting stronger flux exchange between fractures and the matrix. The initial attachment sites of biomass also play a critical role in controlling permeability and flux exchange. It was concluded that fracture-matrix interactions significantly affect biofilm growth patterns, and ignoring these interactions may lead to an incomplete understanding of biofilm dynamics in subsurface systems. The model can be extended to applications such as bioremediation, geological carbon storage, and energy recovery.

5. Diffusive mixing and non-Fickian transport

Yuhang Wang, from China University of Geosciences (Wuhan), discussed the diffusive interactions between hydrogen and cushion gases, which are critical for underground storage applications as they have a great impact on the purity of hydrogen stored in the subsurface porous media. It is crucial to understand the diffusive mass transfer and its impact on the purity of produced hydrogen. This study presents the first quantitative measurements of the diffusive process between the binary system using Raman spectroscopy (Wang et al., 2025b). A generic correlation was proposed to accurately predict the diffusion coefficient between hydrogen and cushion gases under typical storage conditions. Notably, the diffusion coefficient exhibits a linear scaling with the ratio of temperature to cushion gas viscosity in the logarithmic scale. Using the measured diffusion coefficients, the cyclic injection and production processes relevant to underground hydrogen storage are simulated at field-scale. Results suggest that the dispersive mixing plays a role in the purity of the produced hydrogen.

Zhongxia Li, from China University of Geosciences (Wuhan), gave a presentation on mechanisms and quantitative characterization of non-Fickian transport in karst conduits. He presented a comprehensive study on the non-Fickian transport behavior of solutes in rough-walled karst conduits, with a focus on the often-overlooked eddy effect. Through a combination of laboratory experiments and numerical simulations, he systematically investigated how factors such as flow velocity, shape coefficient, and relative roughness influence eddy generation, evolution, and their subsequent impact on solute transport. The study underscores the importance of incorporating vortex dynamics into solute transport models, especially in karst systems, and opens new pathways for upscaling the distributed eddy mobile-immobile model and integrating it with geophysical and hydrochemical methods for field-scale applications. This work provides a critical step forward in accurately predicting contaminant transport and remediation in complex subsurface environments.

6. Thermal and density-driven flow processes

Ke Xu, from Peking University, investigated how overlaying seawater induces thawing dynamics in coastal permafrost via density-driven convection. This topic rises from the accelerating climate change that introduces seawater above high-latitude permafrost along seashore, which may initiate permafrost thawing below 0°C, and thus uncontrollable interaction between subsurface greenhouse gas and the atmosphere. Salt water is of higher density than water at equilibrium with ice. This density mismatch can induce Rayleigh-Darcy convection in melted zone. Experiments show that the ice melting interface is straight and stable at high Rayleigh number conditions, while presents fingering morphology at low Rayleigh number conditions. Numerical simulations demonstrate that this pattern transition is a result of interplay between two flow structures: static convection cell regulated by ice-water interface perturbation, and horizontal convective mixing by classic chaotic Rayleigh-Darcy convection. Dimensional analysis and linear stability analysis confirm distinct Rayleigh number dependencies of these two flow structures and rationalize the observed thawing patterns. More advanced numerical tool is under development to investigate full mechanisms and to provide accurate 3D predictions

Zhao Li, from Hohai University, utilized low-field nuclear magnetic resonance to reveal the thermal impact on clay-rich aquitard permeability. The distributions of transverse relaxation time under different temperatures were detected by low-field nuclear magnetic resonance. The relaxation time, which reflects the mobility of water molecules, is analyzed. The experimental results show that capillary water is the primary water state in saturated clayey aquitard samples, which could flow under specific gradient. The increased movement of capillary water driven by capillary force is the underlying mechanism for thermal effect on permeability of clayey aquitard. The permeability is an exponential function of temperature. The influence of high temperature on discharge is significant. This study contributes to understanding the mechanism of the thermal effect on permeability of clayey aquitard by using the mobility of water molecules.

7. Future challenges

As seen in the editorial, recent advances in microscopic flow and reactive transport have increasingly focused on understanding and modeling complex coupled processes at the pore scale. Key progress has been driven by advanced imaging tools, which allow direct visualization of multiphase flow patterns, CO_2 immobilization pathways, and mineral–fluid interactions. Furthermore, novel experimental and numerical models are improving the characterization of particle clogging, biofilm dynamics, and non-Fickian transport, thereby providing deeper insights into the fundamental mechanisms governing subsurface systems. Despite substantial progress, research still faces numerous challenges.

In one aspect, the accurate modeling of multiphase flow, multi-component transport, and geochemical reactions at the pore scale is crucial for understanding complex processes in porous media. However, developing pore-scale numerical models that simultaneously incorporate these processes, particularly in realistic three-dimensional rock structures, remains a significant challenge. In addition, such pore-scale numerical simulations are often hindered by high computational cost and uncertainties in parameterization, which complicate the reliable upscaling of pore-scale phenomena to core- and field-scale predictions.

In another aspect, pore-scale numerical simulations of CO_2-water-rock reactions have primarily focused on calcite as a single mineral. However, since rocks invariably consist of multiple minerals, achieving efficient and accurate numerical simulation of multi-mineral interactions at the pore scale, particularly for minerals with notably different reaction rates, such as calcite and kaolinite, remains a challenge.

In a third aspect, the current understanding of particle transport in subsurface multiphase systems remains limited. Key challenges include: real-time experimental techniques for observing particle transport dynamics in three-dimensional porous media; the lack of quantitative metrics for particle aggregation effects; and insufficient insight into how fluid-fluid interfaces influence particle transport. Furthermore, the limitations in imaging resolution greatly restrict the ability to accurately and dynamically observe rapid interface evolution and reactive transport processes.

Finally, this field is advancing toward more integrated and predictive multiscale modeling. Future efforts will aim to better upscale pore-scale processes to the core and field scales and further unravel the complex couplings among hydraulic, chemical, thermal, and biological processes. This deeper understanding is essential for addressing emerging challenges in subsurface waste disposal and energy exploitation, such as geological carbon and hydrogen storage, and for improving the management and remediation of underground resources.

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Conflict of interest

The authors declare no competing interest.

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