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Editorial: Pore-Scale Microstructure, Mechanisms, and Models for Subsurface Flow and Transport

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Editorial on the Research Topic

Pore-Scale Microstructure, Mechanisms, and Models for Subsurface Flow and Transport

The microscopic structure of soil, rock and other geological material strongly influences the behavior of groundwater systems, geologic carbon sequestration, and other applications in subsurface flow and transport. Experimental and computational advancements now support a wide range of studies that explicitly link the microscopic structure of materials with both physical mechanisms and larger scale flow and transport behaviors. Predictive pore-scale studies to understand and model displacement and transport rely on geometric information obtained from experimental imaging. As new capabilities are developed, quantitative measurements can be made to inform understanding in a variety of ways. Pore-scale studies can provide insight into the operative mechanisms for particular processes, as well as serving as a tool to directly upscale results from the smaller scale to a larger one. Direct exploration of pore-scale processes have lead to significant contributions toward our understanding of the fundamental physics of flow and transport through porous media. This collection highlights key active research areas and identifies new opportunities to advance the state-of-the art, with representative spectrum of theoretical, experimental and computational contributions.

At the most basic level, high-quality experimental image data is indispensable for pore-scale studies.In recent years, artificial intelligence and machine learning techniques have grown as new tools to improve image data quality. Tawfik et al. compare traditional de-noising technique with a variety of artificial neural networks in the context of application to digital rock physics. This touchstone work assesses the performance for several machine learning approaches and identifies promising avenues for future exploration. Efforts to enhance the fidelity of experimental observations underpin theoretical and computational studies that expand our understanding in many different ways. Soulaine et al. review the state-of-the-art computational microfluidics for geosciences, a emerging modeling approach leveraging microfluidic experiments and high-resolution imaging. After introducing the governing equations and numerical methods used in computational microfluidics, the paper highlights recent success and unsolved challenges in modeling multiphase flow and reactive transport at the pore-scale.

Microscopic imaging techniques provide important opportunities to better understand the energy dynamics of immiscible displacement. Li et al. use microscopic particle image velocimetry (μPIV) to experimentally resolve the dynamics of pore-scale events. This approach provides important information that can help to characterize the bursty dynamics that are typical of two-fluid flow through porous media. Their analysis suggests that as much as 90% of the

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energy of a pore-scale event is reversibly transferred to surface energy, and finding that has important consequences for larger-scale model development. At the macroscopic level, Darcy-scale descriptions of two-fluid through porous media have typically ignored the fluctuations caused by pore-scale events. Rücker et al. consider pressure fluctuations that arise during two-fluid fractional flow experiments. The characteristic energy and time scales are determined and shown to be associated with capillary events that occur within the microstructure. Deeper mechanistic understanding of these phenomena are linked to many possible avenues for research, including as a way to infer wetting phenomena and to formulate a more complete understanding of multiphase flow instabilities and their consequences.

When two-phase flow is capillary or viscous dominated, the relation between total flow rate and pressure drop is linear, similar to the single phase description of Darcy. There is an ongoing effort to classify and describe the transition between these two regimes, a third regime where both capillary and viscous forces are of importance. In Roy et al. the authors use network models to simulate multiphase flow at different flow rates, pore size distributions and fluid saturation fractions. In accordance with earlier research, they observe a power law between flow rate and pressure drop in the transition regime. The authors show how this power law exponent is dependent on pore size distribution and saturation, and obtain a wide range of exponents for different network and saturation settings.

Microscopic insight into CO_2 sequestration is an important application area for microscale studies. Kohanpur et al. present an approach to integrate direct numerical simulation results of pore-scale events into larger domain pore-network models. The modified pore-network model provides better agreement with experimental results of residual trapping of CO_2. Trapping is a key mechanism to reduce the mobility of sequestered CO_2 over short timescales, providing an opportunity for longer-term mechanisms to act. Since the dominant mechanisms for trapping are due to capillary forces subject to the influence of confinement based on the solid microstructure, first-principles studies can provide very important insight into the behavior of real systems.

At even smaller length scales, boundary slip can play a significant role in transport behavior. In the theoretical work of Valdés-Parada and Lasseux, volume averaging techniques are used to derive a generalized model that accounts for the consequences of both Knudsen and diffusive slip contributions in the context of macroscopic dispersion. There are many situations where the length scale for solid microstructure is small enough to constitute an essential contribution to the system behavior. This work is also relevant to cases where solid heterogeneity leads to mass fluxes between sub-micron structures and larger scale structures such as fractions and larger pores. Gouze et al. investigates dispersion processes in porous media. The authors create two sets of porous media samples, both following the same porosity-permeability trends, but with different pore structure evolution and thus dispersion evolution. These two sets allows the authors to investigate how dispersion is affected by micro-structure relative to changes in porosity and permeability. Mass transfer processes also play an important role in surface reactions that can alter the pore structure and cause corresponding changes to macroscropic transport coefficients. Starchenko constructs a first-principles model to study the role played by nucleation in mineral precipitation and growth. The constructed numerical model is used to demonstrate how this mechanism influences the formation of heterogeneous microstructures within a porous material.

The vibrant pore-scale research community fosters essential connections between first-principles physics, high quality experimental data and practical applications. Scientific advancements have always relied on new data sources as a way to substantiate theo retical models and inform engineering applications that benefit society as a whole. As the volume and quality of pore-scale experimental data continue to grow, associated opportunities to learn from theory and computation will grow as well. Insights that result from these developments will be essential to formulate strategic responses to a wide range of challenges that face global society, particularly those related to climate change, water resources management and energy.

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All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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