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# Pore-scale simulation of coupled hydro-geochemical processes and deep learning prediction of permeability

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The quantification and prediction of coupled hydro-geochemical processes in porous media are pivotal for the strategic implementation of a broad range of subsurface projects, including development of petroleum and geothermal reservoirs, geologic carbon sequestration, underground hydrogen storage, contaminant remediation, and mineral extraction.

This work presents a comprehensive numerical study that captures the complex interplay of hydrodynamics and geochemical reactions at the pore scale. This study leverages a robust multi-component reactive transport lattice Boltzmann model (LBM), which accounts for coupled fluid flow, solute transport, and chemical reactions both in the pore fluid and at the pore walls, as well as the evolution of pore geometry due to mineral dissolution and precipitation. It delivers insights into how the microscale structural characteristics of porous media influence transport and reaction pathways. By observing the impact of these processes on porosity and permeability changes over time, the transformation of the physical properties of the porous matrix is delineated.

Further, a deep neutral network is constructed and trained to predict the permeability-porosity relation based on the dataset obtained from the high-fidelity LBM simulations. The trained DNN has high prediction accuracy and strong generalization ability in predicting the permeability–porosity relation (a key input for continuum models) for coupled hydro-geochemical processes but is orders of magnitude faster than the pore-scale LBM simulation.

This investigation not only underscores the intricacies of hydro-geochemical interactions underpinning many subsurface projects but also showcases the powerful synergy between LBM simulations and deep learning. The resulting models and upscaling techniques contribute to predictive and optimizable strategies for long-term efficacy of subsurface projects.