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Pore-scale hydrodynamic evolution within carbonate rock during CO₂ injection and sequestration

Chi Zhang, Siyan Liu, and Reza Barati

University of Vienna, Institute for Meteorology and Geophysics, Vienna, Austria (chizhang@ku.edu)

The continuously rising threat of global warming caused by human activities related to CO₂ emission is facilitating the development of greenhouse gas control technologies. Subsurface CO₂ injection and sequestration is one of the promising techniques to store CO₂ in the subsurface. However, during CO₂ injection, the mechanisms of processes like injectant immobilizations and trapping and pore-scale geochemical reactions such as mineral dissolution/precipitation are not well understood. Consequently, the multi-physics modeling approach is essential to elucidate the impact of all potential factors during CO₂ injection, thus to facilitate the optimization of this engineered application.

Here, we propose a coupled framework to fully utilize the capabilities of the geochemical reaction solver PHREEQC while preserving the Lattice-Boltzmann Method (LBM) high-resolution pore-scale fluid flow integrated with diffusion processes. The model can simulate the dynamic fluid-solid interactions with equilibrium, kinetics, and surface reactions under the reactive-transport scheme. In a simplified 2D spherical pack, we focused on examining the impact of pore sizes, grain size distributions, porosity, and permeability on the calcite dissolution/precipitation rate. Our simulation results show that the higher permeability, injection rate, and more local pore connectivity would significantly increase the reaction rate, then accelerate the pore-scale geometrical evolutions. Meanwhile, model accuracy is not sacrificed by reducing the number of reactants/species within the system.

Our modeling framework provides high-resolution details of the pore-scale fluid-solid interaction dynamics. To gain more insights into the mineral-fluid interfacial properties during CO₂ sequestration, our next step is to combine the electrodynamic forces into the model. Potentially, the proposed framework can be used for model upscaling and adaptive subsurface management in the future.