Pore-scale reactive transport modeling of mineral-water interactions and implications for reaction rate upscaling

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Abstract

The subsurface environment provides a large storage potential for CO₂ and wastes and valuable resources such as water and energy. Sustainable use of subsurface resources and space requires mechanistic understanding and predictive capability regarding the alteration of fractured porous media, which is typically triggered by a series of reactions between mineral phases and chemically reactive fluids. While reservoir scale reactive transport modeling is needed to evaluate system performances, pore scale heterogeneity is also important and should be integrated in large scale analysis. For example, heterogeneity in pore geometry and mineral spatial distribution will largely affect the contact and interactions between minerals and fluids.

In this study, we develop a pore-scale reactive transport model, which captures detailed hydrodynamics and local reactivity that arise from pore-scale geometry and mineralogical heterogeneity. The model is used to simulate geochemical reactions, flow and transport in a representative elementary volume (REV). The simulation results are used to inform continuum scale rock properties (e.g., permeability, reactivity, porosity) using techniques such as local volume average. The upscaling will be based on a set of rules (or database) determined by the pore-scale simulations. This upscaling framework will allow the consideration of local heterogeneity without prohibitively high computational cost, and will improve the performance of reservoir scale reactive transport modeling for applications such as geologic carbon storage and groundwater management.