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Pore scale modeling of reactive flow and transport processes in evolving porous media

Sergi Molins[1]

SUMMARY

The use of subsurface environments in applications related to energy storage and security often involves the injection of fluids that are far from equilibrium with respect to the constituents of the native formation. Such disequilibrium drives geochemical reactions that change the structure of the porous media when primary minerals dissolve and secondary minerals precipitate. This evolution of the medium in turn affects how fluids move in the subsurface leading to emergent behavior that cannot be easily predicted, with both the development of fast flow pathways and the self-sealing of the medium being possible outcomes. The success or failure of the application is thus determined by this non-linear interaction between reactive flow and transport processes.

Historically, the subsurface has been treated as a porous continuum characterized by properties that are applicable over a representative elementary volume that includes both pores and grains. However, the processes that take place at the scale of individual pores and grains may translate into significant impacts at larger scales via nonlinear emergent processes. Over the last decade and a half, characterization and modeling tools applicable at the pore scale have been developed to understand these impacts.

In this talk, I will describe the development of a pore scale model that has been used over the years to understand how heterogeneous pore structures affect effective reaction rates observed at the porous-continuum scale and how the porous media evolves as a result. The model is based on an explicit representation of the interface between solid and fluid. This makes it possible to capture the transport limitations to the rates computed on reactive surfaces. The governing equations are discretized directly on a Cartesian grid using an embedded-boundary (EB) finite volume method using high-order methods. The code solves separately flow, reactive transport, and boundary displacement over a given same time step, assuming that flow and reactive transport solutions change instantaneously as the geometry evolves.

I will illustrate the use of the model with a number of applications, with an emphasis on those that relied on the use of image data obtained from experiments. I will use these examples to discuss the strengths and weaknesses of the pore scale approach in general as well as those associated with this model in particular. In this context, I will contrast it with other models using results from a benchmark problem that was published in 2019. I will conclude by describing ongoing work to address challenges related to capturing physical and mineralogical heterogeneity at a broad range of spatial scales with pore scale and multiscale models, and by identifying future directions in pore scale modeling.

Keywords: Pore-scale modeling, reactive flow, porous media

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[1]Earth & Environmental Sciences Area – Lawrence Berkeley National Laboratory,
1 Cyclotron Road, MS74R316C, Berkeley, CA 94720, USA