Pore-scale and multi-scale models for dissolution in heterogeneous media

SERGI MOLINS[1] DAVID TREBOTICH[2]

[1]Sergi Molins, smolins@lbl.gov
[2]David Trebotich, treb@lbl.gov
Lawrence Berkeley National Lab, Berkeley, CA, USA, 94720

Understanding the evolution of porous media is essential for many subsurface energy applications, including subsurface storage, shale gas production, fracking, CO_2 sequestration, nuclear waste storage, and geothermal energy extraction. Both mineral composition and the intial pore structure of the medium play a significant role in this evolution. Conventional Darcy-scale models treat porous media as a continuum. This approach requires the assumption of well-mixed conditions inside the pore space as well as the use of mechnistic relationships between bulk parameters as the porous medium evolves (e.g. porosity-permeability, porosity-tortuosity). More recently, pore-scale models along with advanced characterization techniques have allowed for accurate simulations of flow and reactive transport within the pore space [1]. However, these models, even with high performance computing, are currently limited in their ability to treat tractable domain sizes [2].

Here we use pore scale modeling to study the evolution of mineralogically and physically heterogeneous porous media as a results of mineral dissolution. We consider scenarios associated with CO_2 sequestration focusing on the dissolution of carbonate minerals under a range of flow conditions in granular and fractured domains. We find that one significant obstacle to modeling this evolution strictly at the pore scale is that it is a multiscale process as changes may take place at spatial scales below the model's resolution. For this purpose, we demontrate two separate muti-scale approaches: one that relies on adaptive mesh refinement that allows to dynamically adjust the resolution of the computatinal grid where needed, and one that builds on our pore-scale approach to add a Darcy-scale continuum description of processes that cannot be captured at a fixed pore scale resolution. Advantages and disasdvantages of each approach are discussed.

[1] Molins S. et al (2014), *Environ. Sci. Technol.*, 48(13), 7453–7460.
[2] Steefel et al. (2013), *Rev. Mineral. Geochem.*, 77(1), 259–303.