

CIVE 6111 Graduate Seminar Series

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Geochemical Reactions: Bridging the Gap between Microscopic and Macroscopic

Monday, November 17, 2014

10:30 am - 11:30 am

Room: D3 W205

Abstract

The pore scale is readily recognizable to geochemists, and yet in the past it has not received a great deal of attention as a distinct scale or environment that is associated with its own set of questions and challenges. Is the pore scale merely an environment in which smaller scale (molecular) processes aggregate, or are there emergent phenomena unique to this scale? Is it simply a finer grained version of the "continuum" scale that is addressed in larger scale models and interpretations? We would argue that the scale is important because it accounts for the pore architecture within which such diverse processes as multi-mineral reaction networks, microbial community interaction, and transport play out, giving rise to new geochemical behavior that might not be understood or predicted by considering smaller or larger scales alone.

The convergence of world-class microscopic characterization and computational software and hardware resources has made it possible to address the problem of subsurface geological carbon sequestration using a new generation of pore scale flow and reactive transport models possessing unprecedented spatial resolution and process fidelity. The high resolution pore scale modeling approach is made possible by the combination of CHOMBO, a DOE SCIDAC developed platform for Navier-Stokes flow and transport within complex geometries, and Crunch, a multicomponent biogeochemical reaction module developed primarily within DOE Laboratories over 20 years. The Chombo code uses an embedded boundary-algebraic multigrid formulation based on a finite volume discretization, with the resulting cut cells accounting for the partial volumes and interfacial geometry of both fluid and

solid. A novel hybrid microscopic characterization approach was developed as part of the Center to take into account both physical and chemical/mineralogical data at multiple length scales, with important contributions from X-ray microtomography, Back Scattered Electron microscopy, and nanoscale FIB-SEM characterization. The hybrid approach has made it possible to map hydrologically accessible mineral reactive surface area at the pore scale within a reservoir sandstone formation at the Cranfield, Mississippi pilot CO₂ injection site. The pore scale maps now serve as the basis for modeling CO₂ solubility and mineral trapping within representative reservoirs.

About the speaker:



Dr. Carl Steefel received his Ph.D. in Geochemistry from Yale University in 1992. He has over 20 years of experience in developing models for multicomponent reactive transport in porous media and applying them to topics in reactive contaminant transport and water-rock interaction. He developed the first routine for multicomponent nucleation and crystal growth in the Earth Sciences (Steefel and Van Cappellen, 1990) and the first multicomponent, multi-dimensional code for simulating water-rock interaction in non-isothermal environments (Steefel and Lasaga, 1994). He has also worked extensively in applying reactive transport modeling to natural systems, including hydrothermal, contaminant, and chemical weathering environments. Recently, he has been involved in experimental studies of cation exchange (Steefel et al., 2003) and mineral dissolution and precipitation (Yang and Steefel, 2008), as well as modeling studies of field systems focused on contaminant transport, microbially-mediated biogeochemical reactions, chemical weathering (Giambalvo et al., 2002; Steefel, 2004; Maher et al., 2009; Li et al., 2009), and isotope systematics (Druhan et al., 2012). More recent work has focused on pore scale studies, including those using high performance computing (Li et al, 2008; Molins et al., 2012).