Rate control in low porosity diffusion-reaction systems

CARL I. STEEFEL[1], SUSAN L. BRANTLEY[2],
ALEXIS K. NAVARRE[3] AND QINHONG HU[4]

[1]Earth Sciences Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley CA 94720, USA (CISteefel@lbl.gov)
[2]Department of Geosciences, Pennsylvania State University, University Park PA 16801, USA (brantley@essc.psu.edu)
[3]Department of Geosciences, Pennsylvania State University, University Park PA 16801, USA (anavarre@geosc.psu.edu)
[4]Chemical Biology and Nuclear Science Division, Livermore National Lab, Livermore, CA 94550, USA (hu7@llnl.gov)

Diffusion-reaction processes in low porosity and permeability rocks have been rarely studied quantitatively. The rate control in these systems, whether by diffusion or by surface reaction, is therefore largely unknown. Such systems can be understood, however, by collecting additional information to constrain the individual dynamic processes. For example, measurement of tracer diffusion rates in the low porosity material makes it possible to uniquely constrain *in situ* integrated reaction rates given a set of elemental or mineralogical spatial profiles. Alternatively, the system can also be constrained uniquely given a knowledge of the position of reaction fronts as a function of time and their thickness, since the reaction front thickness indicates the ratio of the reaction rates to the diffusion rate.

Such systems may be further complicated by reaction-induced porosity and permeability change. If the porosity and permeability are enhanced sufficiently by reaction, then flow can occur where the porosity of the rock has increased, thus resulting in a system with more than one transport mechanism. It is also possible in many cases that diffusion-controlled reaction fronts require the enhancement of porosity via reaction to advance at all. The fact that fronts for minerals with different dissolution rate constants often coincide closely in space may be an indication that the rate of porosity enhancement is controlling the rate of front propagation. These questions are addressed through a combination of multicomponent reactive transport modeling, microscopic mineralogical and elemental characterization, and experimentation.