Multiple approaches to studying diffusion processes in geological media

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The current conceptual model of contaminant transport in unsaturated fractured rock has water moving through fractures, with migration of the entrained contaminants being retarded by diffusion into and within the rock matrix. The diffusion coefficient is implicitly assumed to have a constant, scale-invariant value. However, rocks whose pores are poorly interconnected are known to have anomalous transport properties that strongly impact long-term net diffusion. Complementary and intergrated experimental/modeling approaches are pursued to study diffusion processes in geological media:

(1) Imbibition (analogous to diffusion) tests wherein the water uptake is monitored over time, with the slope of log imbibed water mass versus log time indicative of the pore connectivity of the rock matrix. Change in the slope (if any) can be related to the correlation length of percolation theory.

(2) Gas diffusion experiments, employing an on-line quadrupole gas mass spectrometer to measure real-time trace gas concentrations, to determine diffusion coefficients at several different sample thicknesses to examine scaling effect.

(3) Laser ablation interfaced with inductively coupled plasma-mass spectrometry (ICP-MS) to measure fine-scale tracer concentration to investigate edge-accessible porosity distribution, which is related to pore connectivity.

(4) 3-dimensional images obtained from the synchrotron microtomography system at the Advanced Light Source are analyzed to obtain tracer iso-concentration surfaces, which are indicative of pore connectivity and cross-over length.

(5) All experiments are modeled via random walks on 3-D lattices with different pore coordination and connectivity.

Results indicate that porespace in many rocks is close to the percolation threshold, and use of standard diffusion models for rock matrices can yield misunderstanding of diffusion process and incorrectly calculated diffusivity values.

The importance of diffusion at the microbe-mineral interface: Electrical double layer effects and the impact on precipitation/dissolution
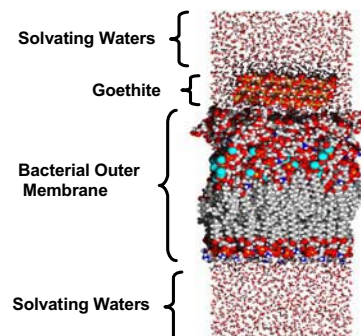
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Understanding the interactions between mineral surfaces and micro-organisms is one of the most challenging areas of research in the geosciences. Many of these interfacial processes take place in very confined spaces and over very short distances where diffusive transport is the predominant process. In this presentation we will give an overview of the surface of the microbial membrane, the chemical factors behind the development of a bacterial electrical double layer, the influence of this double layer on the transport of ions at the surface, and the influence of counter-current diffusion on bacterial mediated precipitation/dissolution reactions.

In the latter case, the chemical microenvironment at the microbial surface is modified by the flux of reactants and microbial byproducts from the organism to the surrounding solution. This flux of reactants is partially controlled by the generally negatively charged microbial surface which induces a cationic flux toward the organism and an expulsion of anions from the surface. These diffusive fluxes can create regions of oversaturation with respect to the mineral precipitation reactions near the microbial surface.

Molecular dynamics simulation of the microbial membrane – mineral interface in a fully solvated system.

Results of both continuum level and molecular dynamics simulations of ion diffusion at microbial surfaces will be presented and the limitations of these approaches in simulating ionic diffusion and at the microbe/mineral interface will be discussed.