

Spreading *versus* mixing effects on reactive transport in groundwater

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Many environmentally important systems involve complex water-rock interactions within natural subsurface systems that exhibit large physical and (bio)geochemical heterogeneity. Contaminant transport and retention are governed by the complex interplay between (bio)geochemical reactions and physical transport along spatially variable water flow paths, where solute dispersion affects the timing, duration, and concentration levels of water contamination arrival downstream of pollution sources.

Longitudinal solute *spreading* among different advective flow paths occurs due to subsurface heterogeneity on various scales, with molecular diffusion and pore-scale dispersion causing also *mixing* of aqueous solutions within flow paths. Combined handling of these different dispersive processes in reactive transport modeling, using a single dispersion or diffusion term, neglects the fact that contaminant *spreading* and solution *mixing* may have very different dispersion effects.

In this study, we consider physical spreading, coupled with precipitation/dissolution and sorption processes, of heavy metals in groundwater downstream of a mill tailings deposit, as one environmentally important example of a multi-component reactive transport system. We use the PHREEQC [1] and LaSAR-PHREEQC [2] modeling approaches to quantify separate and coupled effects of *mixing* and *spreading* on resulting downstream dispersion of reactive contaminants in heterogeneous groundwater systems. Whereas reactions coupled with *mixing* often decrease resulting contaminant dispersion due to formation of reaction fronts, reactions coupled with *spreading* tend to increase the contaminant dispersion through reaction front fingering.

References

- [1] Parkhurst D.L. and Appelo, C.A.J. (1999), *USGS Water-Resources Investigations Report 99-4259*, USGS, Denver, Colorado, USA.
- [2] Malmström M.E., Destouni G., and Martinet P. (2004), *Environ. Sci. Tech.* **38**, 2673-2679.

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Diffusion in mantle and core materials

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Solid-state diffusion is the rate-limiting step in many important geochemical processes in Earth and planetary interiors, especially those involving chemical and isotopic mass transfer among minerals, or minerals and fluids. As the rate-limiting step in creep, diffusion also plays a crucial role in the internal convection and thermal evolution of planets. Experimental and theoretical work on the rates and mechanisms of diffusion in minerals has advanced rapidly, particularly in the last decade. This talk will highlight some of these advances, focusing on work in which the author has been involved.

Experiments on diffusion of lanthanides and actinides in high-Ca pyroxene demonstrate a systematic dependence of the diffusion coefficient on ionic radius and charge for elements that diffuse by a common mechanism. This dependence can be understood in terms of a simple model that considers the elastic energy required to deform the lattice, allowing an ion to jump to an adjacent vacant site. The elastic model provides a useful means for estimating diffusion coefficients of ions that have not been studied experimentally.

Understanding the influence of pressure on diffusion rates is critical for extrapolating diffusion-controlled properties such as viscosity to the conditions of Earth's deep mantle and core. Recent high-pressure experiments on periclase (MgO), close-packed Fe-Ni alloys, and Zn, an analogue for hcp-Fe in Earth's inner core, will be discussed in relation to theoretical approaches for extrapolating diffusion data to high pressures.