Coupled-Process Modeling of a Uranium Bioremediation Field Experiment

STEVEN B. YABUSAKI [1*], YILIN FANG [1], MICHAEL J. WILKINS[1], AND PHILIP E. LONG[2]

[1]Pacific Northwest National Laboratory, Richland, Washington, USA
yabusaki@pnnl.gov,yilin.fang@pnnl.gov, michael.wilkins@pnnl.gov
[2]Lawrence Berkeley National Laboratory, Berkeley, California, USA
pelong@lbl.gov

Field biostimulation experiments at a former uranium mill tailings site are being used to better understand the processes, properties, and conditions controlling engineered bioremediation of uranium contaminated groundwater. A key component of the research is the development of a mathematical model that incorporates three-dimensional variably saturated flow through physically and chemically heterogeneous sediments, as well as the interaction of biologically-mediated reaction products with the subsurface geochemical environment. We present the modeling of the 2008 uranium bioremediation field experiment, in which pulsed acetate groundwater amendment was used to stimulate indigenous metal-reducing bacteria to transform aqueous U(VI) to immobile solid-associated U(IV).

Uranium mobility is sensitive to pH, Eh, alkalinity, calcium, and reactive surface area, as well as aqueous uranium concentrations. In the model, these geochemical conditions are impacted directly by the terminal electron accepting process (TEAP) reactions and indirectly by subsidiary reactions induced by the biologically-mediated reaction products. For example, uranium surface complexation is directly affected by the large amount of bicarbonate produced by the acetate-oxidizing microorganisms but also indirectly by changes in the pH from mineral reactions induced by sulfide. The modeling also addresses site-specific issues such as the continuous influx of actionable levels of U(VI) into the treatment zone, seasonal water table variation, spatially variable physical (hydraulic conductivity, porosity) and geochemical (reactive surface area) material properties, and competition for the acetate electron donor by sulfate reducing bacteria.

Findings include: 1) uranium bioreduction is most effective when acetate concentrations are engineered to exceed the sulfate-reducing bacteria demand; 2) biogenic sulfide promotes the dissolution of Fe(III) minerals leading to an abiotic but biologically mediated Fe(II) source; 3) falling water table sequesters residual reactants and products in the newly unsaturated pores; 4) preferential flow paths for acetate delivery create local zones of enhanced TEAP reactivity and subsidiary reaction; and 5) predicted central metabolic pathway reaction fluxes from a genome-scale metabolic ("*in silico*") model of *Geobacter metallireducens,* correlate well with proteomics data from the field experiment.

The eSTOMP subsurface simulator was used to exploit the large memory and high-performance of massively parallel computers needed to address the high spatial and temporal resolution, large number of reactive species and minerals, and detailed process models.

Cretaceous *P–T–t* evolution of the Fosdick migmatite–granite complex, West Antarctica: orogenic collapse along the East Gondwana margin

CHRIS YAKYMCHUK[1*], FAWNA J. KORHONEN[2], MICHAEL BROWN[1], PHILIP M. PICCOLI[1] AND CHRISTINE S. SIDDOWAY[3]

[1]Laboratory for Crustal Petrology, Department of Geology, University of Maryland, College Park, MD 20742, USA, cyak@umd.edu (* presenting author)
[2]Geological Survey of Western Australia, Department of Mines and Petroleum, East Perth, Australia
[3]Department of Geology, The Colorado College, Colorado Springs, CO 80903, USA

The Fosdick migmatite–granite complex in West Antarctica represents a rare exposure of the anatectic middle crust from along the former active margin of East Gondwana. The complex preserves a polyphase metamorphic history and contains a detailed record of crustal differentiation during a Cretaceous transition from oblique tectonic convergence to divergence across the most long-lived and extensive active plate margin in the Phanerozoic. Migmatites that crop out in the complex preserve evidence of Lower Cretaceous high–*T* metamorphism and anatexis, and subsequent retrograde decompression inferred to record orogenic collapse early during the Upper Cretaceous breakup of the East Gondwana margin. Migmatites collected from the eastern and western extents of the complex contain peak metamorphic assemblages that include garnet, garnet + cordierite or cordierite associated with leucosomes. Sillimanite is preserved as inclusions in garnet, cordierite, and biotite. Phase equilibria modelling constrains prograde heating into the sillimanite + garnet + liquid stability field at temperatures of 850–900°C and pressures of 0.7–1.1 GPa, which was followed by decompression into a cordierite + liquid stability field immediately above an elevated solidus at conditions of metamorphism of temperatures of 850–880°C and pressures of 0.6–0.7 GPa. Melt reintegration along a model isobaric heating path at 0.7 GPa suggests that the metasedimentary protoliths could have produced up to 24 mol.% melt, most of which must have been extracted in order to preserve the garnet– and cordierite–bearing mineral assemblages. This melt was emplaced at higher crustal levels, as represented by Cretaceous peraluminous granites exposed in the periphery of the Fosdick complex—a process that contributed to the differentiation and ultimate stabilization of the East Gondwana active margin now exposed in West Antarctica.

In situ SHRIMP U–Pb isotope analysis of monazite from stromatic metatexite migmatites yield dominantly Cretaceous ages of c. 111–96 Ma. Individual Cretaceous monazite grains show variable zoning patterns in Y and Th, but most contain low-Y cores and high-Y rims. This is consistent with progressive monazite growth associated with garnet breakdown during near-isothermal decompression. These data suggest orogenic collapse and exhumation of the Fosdick complex as a gneiss dome was underway by c. 111 Ma, which supports geophysical studies in West Antarctica and regional studies in the outboard part of the once contiguous margin of East Gondwana that suggest breakup had begun by c. 110–100 Ma.