# Numerical simulation of heterogeneous reactive subsurface

J. BEISMAN[1]*, R. MAXWELL[1], A. NAVARRE-SITCHLER[1], C. STEEFEL[2] AND S. MOLINS[2]

[1]Colorado School of Mines,
1500 Illinois St, Golden, CO 80401
jbeisman@mymail.mines.edu

[2]Lawrence Berkeley National Laboratory,
1 Cyclotron Rd, Berkeley, CA 94720*

Subsurface hydrogeochemical systems, like the critical zone, are the result of dynamic coupled relationships between physical, geochemical, and microbial processes. Reactive transport models provide a quantitative way to evaluate such complex systems. However, parameters and reactions exhibit strong scale-dependence, limiting our ability to extrapolate laboratory results to field systems. We have developed a parallel reactive transport model that allows for numerical simulation of complex, heterogeneous subsurface environments where hydrological, chemical, microbial processes interact. A series of simulations were conducted using ParCrunchFlow to evaluate important interactions between biogeochemical reactions and transport processes in carbon and nutrient cycling in a floodplain setting. These simulations capture the influence of physical and mineralogical heterogeneity on oxygen concentrations in a variably reductive subsurface. Steady state oxygen concentrations in the simulations are low in areas of low hydraulic conductivity and high total organic carbon where microbial reactions result in the reduction of nitrate to ammonia. The second-order explicit Godunov method was used to calculate advection, which minimized numerical dispersion and resolved sharp boundaries and steep gradients at boundaries between high and low permeability zones. These zones are more diffuse when simulated with lower-order advection schemes available in other reactive-transport simulators. Upscaled, effective reaction rates in the floodplain vary with differences in the way permeability and mineralogy are heterogeneously distributed in the subsurface.