

## **Integrated Surface-Subsurface Reactive Transport**

In natural surface-subsurface systems, areas of disproportionately high reaction rates often heavily influence total elemental fluxes. These pockets of high reaction rates tend to occur at interfaces, such as the capillary fringe or hyporheic zone, where a hydrologic flowpath converges with either a chemically distinct hydrologic flowpath or a reactive substrate. Understanding the affects that these highly reactive zones have on the behavior of shallow subsurface systems is integral to the accurate quantification of nutrient fluxes and biogeochemical cycling. The numerical simulation of many of these areas of disproportionately high reaction rates requires an integrated surface-subsurface modeling approach. Here we present recent developments to the massively parallel reactive transport code ParCrunchFlow. This model, previously applicable only to steady-state, saturated subsurface flows, has been extended to transient, surface-subsurface environments, allowing the numerical simulation of reactive transport processes in highly-heterogeneous, field-scale systems. Proof-of-concept simulations involving the biogeochemical cycling of carbon (C) and nitrogen (N) in both hillslope and floodplain settings are presented.

### **Peer Reviewed Publications**

**Beisman, J.**, Maxwell, R., Navarre-Sitchler, A., Steefel, C., Molins, S. ParCrunchFlow: An Efficient, Parallel Reactive Transport Simulation Tool for Physically and Chemically Heterogeneous Saturated Subsurface Environments. *Computational Geosciences*, In Review.

### **Awards**

2013 Edna Bailey Sussman Grant Recipient

### **Conference Presentations**

**Beisman, J.**, Maxwell, R., Navarre-Sitchler, A., Steefel, C., Molins, S. High-resolution reactive transport: A coupled parallel hydrogeochemical model. GSA Annual Meeting, Paper No. 245-27, Denver, CO, October 2013.

**Beisman, J.**, Maxwell, R., Navarre-Sitchler, A., Steefel, C., Molins, S. High-resolution reactive transport: A coupled parallel hydrogeochemical model. AGU Fall Meeting, Abstract H43D-1468, San Francisco, CA, December 2013.

**Beisman, J.**, Maxwell, R., Navarre-Sitchler, A., Steefel, C., Molins, S. High-resolution reactive transport: A coupled parallel hydrogeochemical model. Goldschmidt 2014, Abstract 3232, Sacramento, CA, June 2014.

**Beisman, J.**, Maxwell, R., Navarre-Sitchler, A., Steefel, C., Molins, S. High-resolution reactive transport: A coupled parallel hydrogeochemical model. CMWR 2014, Submission ID 3232, Stuttgart, Germany, June 2014.

**Beisman, J.**, Maxwell, R., Navarre-Sitchler, A., Steefel, C. Implementation of positivity-preserving, high order advection schemes in a reactive transport model. AGU Fall Meeting, Abstract H41F-0898., San Francisco, CA, December 2014.

### **Workshops**

Participant, Expanding the Role of Reactive Transport Modeling within the Biogeochemical Sciences Workshop, Alexandria, VA, April, 2014.