

## Thermokinetic simulation of microbial respiration and dissolution precipitation reactions of minerals

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Microbial processes interact closely with abiotic geochemical reactions and mineralogical transformations in several hydrogeochemical systems. Reactive transport models are aimed to analyze these complex mechanisms involving degradation of organic matter by successive terminal electron acceptors (TEAPs) mediated by microbes through the continuum of unsaturated zone (soil) – saturated zone (aquifer).

The new rate law of microbial respiration in various geochemical environments proposed by Jin & Bethke [3] were used to simulate reactive transport of nitrate and organic matter in the framework of the concept of an artificial recharge of aquifer. On the other hand, the generalized rate law of mineral dissolution – precipitation reactions derived from the transition state theory TST [4] were used for dissolution – precipitation of silica, aluminosilicate, carbonate, oxyhydroxide, and sulphide minerals. The kinetic parameters are compiled from the literature measurements based on laboratory constrained experiments and field observations. Numerical simulations, using the geochemical software PHREEQC [1] were performed aiming to identify the key reactions mediated by microbes. In this numerical modelling we have explicitly accounted for interactions between microbiological reactions and geochemical processes according to the two-step partial equilibrium approach (PEA) for the overall reaction of organic matter degradation [2].

The Jin and Bethke [3] approach combining reaction kinetics and biogeochemical thermodynamic constraints is successfully applied to denitrification experiments in the presence of acetate and pyrite conducted in the laboratory for batch and column systems. The parameters used/fitted for this laboratory modelling is thus extended to simulate the denitrification processes in a field case where acetate and FeS<sub>2</sub> are the electron donors and O<sub>2</sub>, NO<sub>3</sub>, Fe(OH)<sub>3</sub>, SO<sub>4</sub> are the electron acceptors in the framework of a continuum UZ – SZ aiming to identify the stabilized redox zones. The detailed results obtained on two actual case studies will be presented.

- [1] D. L. Parkhurst & C. A. J. Appelo, (1999) *Wat. Resour. Investigations Report*. 99-4259, U. S. Geol. Survey.  
 [2] A. Brun, P. Engesgaard, T. H., Christensen & D., Rosbjerg (2002) *J. Hydrol.* **256**, 230-249.[3] Q. Jin & C. M. Bethke (2007) *Am. J. Sc.* **307**, 643-677. [4] C. Lasaga (1984) *J. Geophys. Res.* **89**, 4009-4025.

## Inferring phosphorus dynamics in flow through lakes from sediment biogeochemistry

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In a study of regime changes in Muskegon Lake, Michigan, USA (a flow through lake) relationships were identified between diatom communities and sediment phosphorus (P). Diatoms and P concentrations are often used to infer historical P loadings and trophic status in lakes. In flow through lakes, linking these measurements to P dynamics (e.g., burial, release, outflow concentrations) has been difficult because additional indicators of process(es) are required and relationships between diatom communities and P to infer process(es) have not been well established.

In the Muskegon Lake study, major and trace element data were combined with diatom community structure data. We observed that the abundance of *Aulacoseira granulata*, a common freshwater diatom, has an inverse relationship with sediment P while geochemical proxies (e.g. P, Ca, Fe, Al, and Mn) have similar profiles until the onset of human disturbance (~1850) where they became decoupled at varying rates. We hypothesized that the inverse relationship between P and *A. granulata* in the core is related to regime shifts in available P. If true, this relationship should also occur in modern day flow through lakes.

To test this hypothesis, two modern flow through lakes, Morrow Lake, Michigan, USA and Lake Allegan, Michigan, USA, were examined by analyzing inlet and outlet water column major and trace elements and diatom populations. These lakes showed a link between water column P availability and *A. granulata*. Lake Allegan sequestered 6,800 kg P/growing season and exhibited a reduction in *A. granulata* abundance from 48% (inflow) to 16% (outflow). Morrow Lake released 2,500 kg P/growing season and showed an increase in *A. granulata* abundance from 0% (inflow) to 48% (outflow). While these results were consistent with the hypothesis, the specific mechanisms require further investigation.

Inferences developed in this study have led to a better understanding of biogeochemical processes dictating P source/sink dynamics. Further implications for this work include insight for environmental recovery expectations.