Modeling reductive dissolution of iron oxides and associated arsenic mobility under varying organic electron donor loads

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Millions of individuals worldwide are chronically exposed to hazardous concentrations of arsenic from contaminated drinking water. Despite massive efforts towards understanding the extent and underlying geochemical processes of the problem, numerical modelling and reliable predictions of future arsenic behaviour remain a significant challenge. One of the key knowledge gaps concerns a refined understanding of the mechanisms that underly arsenic mobilization and the quantification of the factors that affect this process. In this study we focus on developing and testing of appropriate numerical model approaches to represent the microbially mediated reductive dissolution of iron oxides and the concomitant release of sorbed arsenic.

The initial model development was guided by data and hypothesized processes from a previously reported well-controlled column study [1] in which arsenic desorption from ferrihydrite coated sands by variable loads of organic carbon was studied.

The reaction network that was implemented into the reactive transport code PHT3D [2] simulates the reductive dissolution of ferrihydrite and associated iron phase transformation processes, which showed to play an integral part for arsenic mobilization and retention. It captures the impact of variable organic carbon loads and the corresponding increases in the rate of reductive dissolution of ferrihydrite and increased levels of arsenic mobilization. In addition the model simulations successfully reproduce the lab-observed iron phase transformations and the impact of these transformations (e.g., ferrihydrite to magnetite) on variations of arsenic sorption capacities and the associated arsenic mobility.

[1] Tufano and Fendorf (2008) *Environ. Sci. Technol.* **42**, 4777-4783. [2] Prommer *et al* (2003) *Ground Water* **41**(2), 247-257.