The Effect of Transport Heterogeneity on Redox Reaction Rates at the Pore and Continuum Scale

Objectives

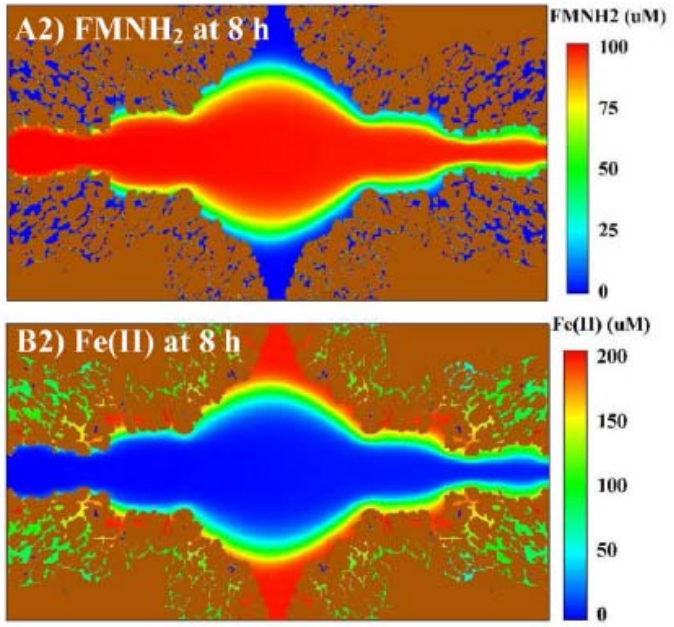
- To evaluate the effects of subgrid heterogeneity on the modeling of redox reactions in natural materials with complex pore structures.

Approach and Results

- A micromodel, representing a numerical grid in a continuum model, was fabricated in EMSL with pore features similar to natural porous media.
- Pore surfaces were coated with Fe(III) oxide, a common electron acceptor for biogeochemical reactions.
- A biogenic reactant (flavin) was run through the system and spatially distributed reaction progress over time was followed by optical measurements and spectroscopy.
- Complex reaction patterns and spatially variable kinetic rates were observed that were controlled by the distribution of advective and diffusive transport pathways.

Significance and Impact

- Results supported the development of a general, domain-based scaling approach to predict redox reaction rates in heterogeneous natural porous materials over a large range in spatial scales.



Micromodel reactants ($FMNH_2$) and products (Fe(II)) after 8 h. Flow is from left to right.

Liu, Y., Liu, C., Zhang, C., Yang, X, and Zachara, J,M. (2015) Pore and continuum scale study on the effect of subgrid heterogeneity on redox reaction rates. *Geochimica et Cosmochimica Acta*, **163**, 140-155. doi:10.1016/j.gca.2015.04.039.