Subgrid Domain Approach for Scaling Reaction Rates in Heterogeneous Subsurface Materials

Objective

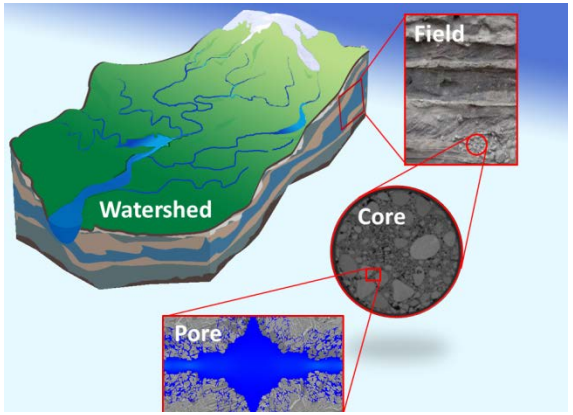
- Evaluate the effect of subgrid physiochemical heterogeneity on reaction rates.
- Develop an approach based on non-reactive tracer behavior to scale reaction rates in subsurface materials.

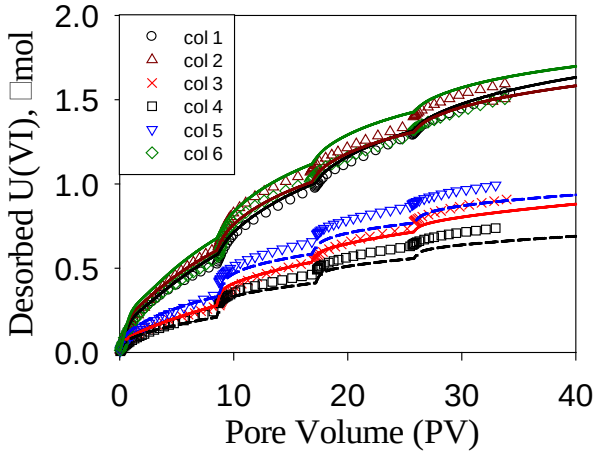
Approach/Results

- Column experiments to evaluate grain-scale reactions under flow conditions in sediments with heterogeneous distribution of physiochemical properties using U(VI) desorption as an example.
- The effective rate of U(VI) desorption varies significantly in the same material, but with different subgrid heterogeneity.
- Subgrid domain model developed from non-reactive tracer transport behavior can effectively scale reaction rate without modifying reaction parameters.

Significance and Impact

- Bridge models of geochemical and biogeochemical reaction rates and reactive transport from the fine to large scales.
- Minimize the uncertainties of model predictions in heterogeneous porous media.
- Leads to direct application of mechanism-based rate expressions without modifying reaction rate parameters in macroscopic systems.





Subgrid heterogeneity in physiochemical properties is ubiquitous in subsurface materials (top); subgrid heterogeneity poses a major challenge in scaling reaction rates, and subgrid domain model significantly improves model prediction (bottom)

•Liu C, J Shang, H Shan and JM Zachara (2014) "Effect of subgrid heterogeneity on scaling geochemical and biogeochemical reactions: A case of U(VI) desorption." *Environmental Science & Technology,* 48( ), 1745-1752. DOI: 10.1021/es404224j