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ABSTRACT TITLE: Development of Reaction-based Process Models for Complex Subsurface Systems

ABSTRACT: Geochemical and biogeochemical processes occur fundamentally at the pore-scale that can be described using reaction-based models. A major challenge to develop reaction-based process models for complex subsurface systems is that reaction rates and other parameters change as they are extrapolated from the pore to large scales. The scale-dependent behavior is caused by the heterogeneous distribution of reaction properties including sediment surface area/reactivity, microbial community assemblage and enzymatic functions, and transport properties that affect the supply and removal of reactants and/or reaction products. While large scale heterogeneity such as geological formations and facies may be explicitly considered in a reactive transport model, subgrid heterogeneity that is often below characterization resolution is a major source of model prediction uncertainty. In this poster, we will present approaches to scale reaction properties measured in the laboratory for field scale applications, and to minimize model prediction uncertainties caused by subgrid heterogeneity. The U(VI) sorption/desorption process in Hanford 300A sediments will be used as an example.

A set of column experiments with different sediment packing structures to mimic field scale subgrid heterogeneity were performed, and the experimental results were used to evaluate scaling approaches. A statistical approach based on grain-size distribution was developed to estimate field-scale reaction properties and their uncertainty including sediment surface site concentration/reactivity, organic carbon content and microbial respiration rates, and U(VI) sorption/desorption rate constants. The reaction properties in sediments are assumed to correlate with grain size distribution and be linearly additive with respect to grain size mass fractions in this approach. Once the reaction properties are determined for individual grain size fractions, the reaction properties at the field-scale can be estimated from the grain-size distribution data, which are easier to obtain than the reaction properties. Comparison of model simulations with experimental results indicated that a sub-grid, multi-domain treatment of reaction properties can further reduce the prediction uncertainties caused by subgrid heterogeneity of hydrological properties. The result was confirmed using a micromodel experiment with in-situ measurements of reaction rates in heterogeneous porous media under variable flow conditions. The presentation will also discuss the future extension of scaling concepts and approaches to the development of reaction-based biogeochemical models for microbially mediated organic carbon degradation and CO_2 production in complex field systems.

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