Upscaling biogeochemical reaction rates in heterogeneous porous media: Reactive transport modeling approaches

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The heterogeneity of subsurface environments poses daunting challenges in understanding biogeochemical reactions in porous media. Reactive transport models, which integrate physical, chemical, and biological processes, can serve as powerful tools to quantitatively evaluate the impact of heterogeneity on various biogeochemical processes. Here, the effect of pore architecture and connectivity on upscaled reaction rates was investigated using reactive transport models across multiple spatiotemporal scales. First, the effect of spatial permeability variations on upscaled chemical weathering rates was evaluated at the column and field scales. Numerical simulation results illustrated the depletion of the reactive mineral surface along the fast flow paths while the mineral surface in stagnant regions was preserved over thousands of years. As a consequence, surface area normalized weathering rates were significantly underestimated compared to the rate measured in a well-mixed laboratory condition. Next, pore scale reactive transport simulations were carried out to study the effect of heterogeneous biomass distribution on upscaled reaction rates. The large influence of pore scale heterogeneity on the first-order consumption reaction kinetics was identified under fast flow and reaction conditions. These conditions also strengthened the effect of uneven microbial distribution leading to increased errors of upscaled rate estimates.