Physical heterogeneity controls on geochemical reaction rates

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Physical heterogeneity in geologic systems induces spatially variable fluid and solute transport rates, which can lead to spatially variable geochemical behavior. Our understanding of coupling of physical heterogeneity and geochemial behavior is limited, however. Reactive transport models allow for exploration and elucidation of the coupling of physical heterogeneity and geochemical rates.

In this study we present results from reactive transport simulations of anorthite dissolution in a spatially heterogeneous permeability field. Simulations were performed with the reactive transport code CrunchTope on a 2 m x 2 m grid with 2 cm grid discretization. Permeability distributions were generated with sequential Gaussian simulation with log normal distribution around a geometric mean of permeability of 10^{-13} m^2 and geometric variance of the natural log of permeability ($\sigma \ln k$) of 5.3 and 26.5 to represent varying degrees of heterogeneity. Distributions with isotropic structure and anisotropic structure were created to add effects of layered heterogeneity to the analysis. Fifty realizations of 14 different permeability cases were generated and imported into the reactive transport simulation for 701 total simulations. An additional model with homogeneous permeability of 10^{-13} m^2 was included for comparison.

Simulated mineral dissolution rates mapped onto surface-controlled, transport-controlled, and saturation-state-controlled regions that provide insight into local reaction rates (each cell) and effective reaction rates (flux weighted concentrations for the domain). Surface-controlled regions occurred at highest flow velocity where solute concentrations remained low. Transport-controlled regions, where reaction rates scaled with velocity, were limited. The largest portions of the domain comprised reaction rates that were controlled by inherited equlibrum of the fluids from upstream reactions, highlighting the importance of thermodynamics on reactive transport. Results of the study show that highly anisotropic permeabilty fields with $\sigma \ln k = 5.3$ induce preferential flow in the domain that results in a enhancement in effective mineral dissolution rates compared to the homogeneous case. Increased variance to $\sigma \ln k = 26.5$ results in large, non-reactive areas of the domain due to the strong preferential flow that reduces effective dissolution rates.