Upscaling Reactive Transport using Multi-Rate Mass Transfer

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ABSTRACT: Fast chemical reactions are driven by mixing-induced chemical disequilibrium. In porous media mixing is poorly represented by the advection dispersion equation (ADE). Instead, effective dynamics models, such as Multi-Rate Mass Transfer (MRMT), have been successful in reproducing observed field scale transport, notably breakthrough curves (BTCs) of conservative solutes. We study whether such effective models, derived from conservative transport observations, can be used to describe effective multicomponent reactive transport in heterogeneous media. We use a localized formulation of the MRMT model that allows us to solve general reactive transport problems. We test this formulation on a simple three species mineral precipitation problem at equilibrium numerically. We find an excellent agreement between the two models in terms of cumulative precipitated mass for a broad range of generally stationary heterogeneity structures. We compare additionally the concentration variability of the heterogeneous simulation with the variability in mobile and immobile concentrations of the MRMT model. Our results indicate that mass transfer models can be considered to represent quite accurately the large scale effective dynamics of mixing controlled reactive transport.