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Non-local in time formulations for reactive transport

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The rate at which equilibrium chemical reactions occur is driven by mixing-induced chemical disequilibrium. At the field scale, mixing is poorly represented by an Advection Dispersion type equation (ADE). Instead, non-local in time variants have been proposed to represent effective transport dynamics. These include formulations such as the Multi-Rate Mass Transfer (MRMT) or Continuous Time Random Walk (CTRW) methods, which have been successful in representing breakthrough curves (BTCs) of conservative solutes at intermediate scales. The original formulation of these equations is not amenable to reactive transport, which requires local (in space and time) concentrations. However, such original formulations can be easily localized, which allows using these formulations for general solutions. The objective of our work is, first, to test whether non-local transport models derived from conservative solutes observations, can be used to describe effective reactive transport in heterogeneous media. To this end, we use a numerical approach to obtain the spatial and temporal distribution of mineral precipitation in a binary system at equilibrium in a heterogeneous aquifer. We then compare these reaction rates to those corresponding to an equivalent (i.e. same conservative BTC) homogenized media with transport characterized by a non-local in time equation involving a memory function (MRMT). We find an excellent agreement between the two models in terms of cumulative precipitated mass, and depending on the local heterogeneous structure the match is acceptable for the reaction rate. These results indicate that mass transfer models are an excellent tool for upscaling mixing controlled reactive transport.