Upscaling bimolecular reactive transport with mixing-limitation: Ephemeral ballisticity

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The challenge of determining mixing extent of solutions undergoing advective-dispersive-diffusive transport is well-known. In particular, reaction extent between displacing and displaced solutes depends on mixing at the pore scale, that is generally smaller than continuum scale quantification that relies on dispersive fluxes at the representative elementary volume scale. Here a novel mobile-mobile mass transfer approach is developed to distinguish diffusive mixing from dispersive spreading in one-dimensional transport involving small-scale velocity variations with some correlation, such as occurs in hydrodynamic dispersion, in which short-range ephemerally- ballistic transports give rise to dispersed but not mixed segregation zones. When considering transport of a single solution, this approach distinguishes self-diffusive mixing from spreading, and in the case of displacement of one solution by another, each containing a participant reactant of an irreversible bimolecular reaction, this results in time-delayed diffusive mixing of reactants. The approach generates models for both kinetically-controlled and equilibrium irreversible reaction cases, while honoring independently measured reaction rates and dispersivities. The mathematical solution for the equilibrium case is a simple analytical expression. The approach is applied to published experimental data on bimolecular reactions for homogeneous porous media under post-asymptotic dispersive conditions with good results.