

A Transition in the Cumulative Reaction Rate of Two Species Diffusion with Bimolecular Reaction

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Diffusion and bimolecular reaction between two initially separated reacting species is a prototypical small-scale description of reaction induced by transverse mixing. It is also relevant to diffusion controlled transport regimes as encountered in low-permeability matrix blocks in fractured media. In previous work, the reaction-diffusion problem has been analyzed as a Stefan problem involving a distinct moving boundary (reaction front), which predicts that front motion scales as \sqrt{t} , and the cumulative reaction rate scales as $1/\sqrt{t}$. We present a general non-dimensionalization of the problem and a perturbation analysis to show that there is an early time regime where the cumulative reaction rate scales as \sqrt{t} rather than $1/\sqrt{t}$. The duration of this early time regime (where the cumulative rate is kinetically rather than diffusion controlled) depends on the rate parameter, in a manner that is consistently predicted by our non-dimensionalization. We also present results on the scaling of the reaction front width. We present numerical simulations in homogeneous and heterogeneous porous media to demonstrate the limited influence of heterogeneity on the behavior of the reaction-diffusion system. We illustrate applications to the practical problem of in-situ chemical oxidation of TCE and PCE by permanganate, which is employed to remediate contaminated sites where the DNAPLs are largely dissolved in the rock matrix.