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

Chemical oxidation of dense nonaqueous-phase liquids (DNAPLs) by permanganate has emerged as an effective remediation strategy in fractured rock. Little is understood about the behavior of simultaneous reaction and diffusion of DNAPL and chemical oxidant in porous bedrock. This system was modeled using 1-D homogeneous numerical model. Under fast reaction conditions, a stable, sharp, moving reaction front was observed. A semi-analytical solution was developed which simulates the propagation of this reaction front. The reaction front was shown to propagate as the square-root of time, indicating that it is a diffusive process. So far it was believed that the cumulative reaction rate within the bedrock exhibits a decreasing $(1/\sqrt{t})$ behavior with time for bimolecular reactions. However, the results of numerical calculations for this problem shows that there exist an early time regime during which the diffusion is dominant and the cumulative reaction rate is increasing with time. The early time regime can be thought as a time before which the reaction front has formed. So we may expect that for relatively slow reactions it takes more time for reaction front to form and in some cases it may affect the process of remediation. Our analytical calculations based on perturbation analysis for early time regime also indicated that the cumulative reaction rate during the early time regime is increasing as $\sqrt{t}$ with time.