A Practical Modeling Tool to Estimate Cleanup Timeframes in Highly Heterogeneous Aquifers with Matrix Diffusion and Degradation Reactions

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Background/Objectives. Although advection-dispersion equation (ADE) models are frequently applied to estimate cleanup timeframes as part of remedy evaluation and selection, many field and laboratory studies indicate that the ADE fails to capture the frequently observed long tails of contaminant concentration versus time in monitor well data. This inability of the standard (deterministic) ADE to accurately simulate tailing can potentially lead to a significantly underestimated cleanup timeframe with actual observed contaminant concentrations remaining for longer periods of time at levels above cleanup goals. Given the success of the continuous time random walk (CTRW) modeling framework in capturing observed tailing in many field and laboratory studies, this paper presents a generalized ADE model using CTRW theory that simulates heterogeneous advection, sorption, matrix diffusion, and sequential first-order reactions of both parent (e.g., TCE) and its degradation products (e.g., cis-1,2-DCE and VC). This new modeling tool is expected to be useful for improving estimates of the cleanup timeframe particularly during the monitored natural attenuation (MNA) remedial component of long-term site management.

Approach/Activities. Given the inability to fully characterize the variability in subsurface permeability and diffusion coefficient values in highly heterogeneous mobile and immobile zones even with high resolution site characterization tools, both advection and matrix diffusion are represented stochastically using a generalized ADE. This new extension of the ADE uses probability density functions to represent contaminant transport in the mobile and immobile zones. New analytical solutions are developed and solved semi-analytically in order to compare estimated cleanup times using these generalized ADE model solutions with standard mobile-immobile ADE models with first-order reaction. As a case study example, this new CTRW modeling tool is then applied to estimate the cleanup timeframe of both parent (TCE) and its degradation products (cis-1,2-DCE and VC) based on the observed long tails of slow decreasing concentrations over time in monitor well data at the Harris CERCLA site in Palm Bay, Florida.

Results/Lessons Learned. Consistent with many other studies of the ADE, results of this study indicates that ADE mobile-immobile models may under-predict the cleanup timeframe particularly when degradation rates are low. This inability of the ADE to accurately represent tailing indicates that standard ADE-based models may not be useful tools for simulating the cleanup time frame particularly in highly heterogeneous aquifers with low degradation rates. The generalized ADE model in this study a natural extension of the standard ADE and is parsimonious with only a few model parameters that can be measured in the field. Effects of preferential advective transport in highly heterogeneous mobile zones is represented using a heterogeneity parameter (β), which can be estimated from the variance of hydraulic conductivity measurements or from the slope of log C versus time in tracer test breakthrough curve data. Given that this CTRW model is easy to use and is based on a theoretically consistent mathematical framework, the extension of this practical modeling tool to include adsorption-desorption, matrix diffusion, and mass destruction via first-order sequential first-order reactions is expected to be particularly useful for improving estimates of the cleanup timeframe for MNA remedies as part of long-term site management.