A New Modeling Tool to Estimate Cleanup Rates in Highly Heterogeneous Aquifers with Matrix Diffusion and Time-Dependent Source Mass Flux

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Background/Objectives. With the advent of high resolution site characterization (HRSC) tools, it is now known that most sites are highly heterogeneous with mobile contaminants moving along preferential transport pathways particularly when the variance of hydraulic conductivity measurements is greater than one. In addition to heterogeneous advection, contaminants also diffuse into nearby low permeability silt and clay immobile zones with slow back-diffusion rates into the mobile zones. For plume transport in heterogeneous mobile and immobile zones, the standard ADE can fail to capture the frequently observed long tails of contaminant concentration versus time in monitor well data leading to significantly underestimated cleanup timeframes. Based on the success of the continuous time random walk (CTRW) modeling framework in capturing observed tailing in many field and laboratory studies, this paper presents an extended ADE model 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). New analytical solutions are presented that can simulate effects on downgradient plume concentrations as a result of changes in source mass flux over time from either natural source zone depletion (NSZD) or active source zone remediation.

Approach/Activities. Because of the inability to fully characterize the variability in subsurface permeability and diffusion coefficient values in highly heterogeneous mobile and immobile zones even with HRSC 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. The key parameter for the extended model is the power law exponent (β) of the travel time function, which is shown to be related to the variance of hydraulic conductivity data measurements. 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. Results of this study indicates that standard ADE models may under-predict both the cleanup rates and overall cleanup timeframe particularly when degradation rates are low. The extended ADE (CTRW) model in this study is a natural extension of the standard ADE and is parsimonious with only a few model parameters that can be measured in the field. Both mobile and immobile zone concentrations can be estimated for comparison with field data. This extended ADE model is easy to use and is applicable for adsorption-desorption, matrix diffusion, and mass destruction via first-order sequential first-order reactions. With the extension of this modeling framework for time-dependent source releases, this modeling tool is expected to be particularly useful for improving estimates of the MNA cleanup timeframes of large dilute plumes as part of long term site management.