Effects of Heterogeneity and Back-Diffusion on Cleanup Timeframe

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Background/Objectives. As shown in high resolution site characterization (HRSC) studies, most sites are highly heterogeneous with mobile contaminants moving along preferential transport pathways particularly when the variance of hydraulic conductivity is greater than one. In addition to heterogeneous advection, contaminants also diffuse into heterogeneous immobile zones with a wide spectrum of back-diffusion rates into the mobile zones. For plume transport in heterogeneous aquifers in which reactive mixing is limited, the standard ADE can both over-estimate reaction rates and fail to capture the frequently observed long tails of contaminant concentration versus time leading to underestimated cleanup timeframes. Building on the success of the continuous time random walk (CTRW) modeling framework in capturing observed tailing in many field and laboratory studies, this paper applies an extended ADE model (HET-TRANS) to examine the effect of mobile and immobile zone heterogeneity on cleanup times in highly heterogeneous aquifers. This extended-ADE model simulates heterogeneous advection, sorption, matrix diffusion, and sequential first-order reactions of both parent and degradation products of chemicals including chlorinated VOCs and PFOA.

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, both advection and matrix diffusion are represented stochastically using a generalized ADE. This extended ADE model uses probability density functions to represent contaminant transport in the mobile and immobile zones. This allows one to simulate pore-scale processes that occur below the resolution of numerical model grids. The key parameters for the extended ADE model are the variance in hydraulic conductivity of the mobile and immobile zones, volume fraction of the immobile zones, porosity of the immobile zones, and different degradation rates in the mobile and immobile zones. Sensitivity analyses are needed to better understand effects of these parameters on the estimated cleanup timeframe.

Results/Lessons Learned. Results of this study indicate that standard ADE models, which assume homogeneous media, may under-predict the cleanup timeframe. Sensitivity analyses show that in an increased heterogeneity in mobile and immobile zones cause increased tailing leading to a longer cleanup timeframe. Sensitivity analyses also show that the immobile zone degradation rate has an important effect on plume tailing, which can especially be important for slowly degrading compounds such as PFOA, 1,4 dioxane, and chlorinated solvents. Because the standard ADE assumes perfect mixing in mobile and immobile zones, it overestimates reaction rates that decrease tailing leading to an under-estimated cleanup time. As expected, a higher immobile zone volume fraction will cause a longer cleanup time frame because of greater storage of contaminants in immobile zones.For each of these key model input parameters, spatial plots of concentration versus distance from the source are also presented to help examine zones where back-diffusion may control the cleanup timeframe.