

Matrix Diffusion Modeling: Handling Heterogeneity

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Background/Objectives. Restoration at current and former military installations is expected to cost the U.S. Department of Defense (DoD) more than ten billion dollars. Many of these sites contain groundwater that is contaminated by chlorinated volatile organic compounds (CVOCs), often in the form of dense non-aqueous phase liquids (DNAPLs). DNAPLs serve as concentrated sources of groundwater contamination from which most dissolved CVOC plumes originate. Unfortunately, some CVOC sites have proven to be exceedingly difficult to address due to the phenomenon of matrix diffusion. This process may occur in any heterogeneous setting, but it is particularly important in certain fractured bedrock sites, and in sites with extensive clay lenses or layers. These types of complex site conditions tend to produce plumes that are long lived, requiring extensive long-term monitoring.

To better equip the groundwater community with cost-effective, accessible, useable, and practical tools for addressing CVOC contamination in complex fractured and heterogeneous environments, the DoD's Environmental Security Technology Certification Program (ESTCP) has funded the development of the REMChlor-MD Toolkit.

Approach/Activities. REMChlor-MD allows for efficient modeling of matrix diffusion in aquitards, layered and heterogeneous systems, and rock systems with parallel fractures. The tool provides two options for estimating heterogeneity at a site: a Simple Heterogeneity Calculator (Tier 1) and an Advanced Heterogeneity Calculator (Tier 2). The Tier 1 option provides Users with simple pictograms for selecting simplified conditions that best match their site. The Advanced option allows users to apply site-specific data from up to four boring logs to estimate the fraction of transmissive zone volume influenced by matrix diffusion, the average length of the diffusion, and the surface area of the transmissive zone-low permeability zone interfaces.

Results/Lessons Learned. Heterogeneity at contaminated groundwater sites that causes matrix diffusion can be quantified using simple algorithms that supply data to the new REMChlor-MD code. Based on boring log information, the two-Tier Heterogeneity Calculator will allow users to easily incorporate key geologic and stratigraphic information into their REMChlor-MD groundwater transport models. Currently being beta-tested, the easy-to-use and free REMChlor-MD Toolkit will be publicly available in the summer of 2018.