Pre-Proposal

Determining Kinetic Parameters for Improved Modeling of the Carbon Tetrachloride Soil-Vapor Extraction Process

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Introduction

Current models for carbon tetrachloride in the Hanford Site vadose zone use an assumption of equilibrium partitioning to simulate the soil-vapor extraction (SVE) process. Current differences between the simulated and observed SVE yields are strongly related to this assumption. The simulations do not account for any rate-limited (kinetic) interfacial mass transfer effects because there are no data available to effectively model the SVE process in this way. Thus, current models do not effectively simulate the observed SVE results. An updated kinetic-based model for SVE is needed to improve history matching simulations that support the conceptual model of carbon tetrachloride in the vadose zone at the Hanford Site and to provide a more representative model to evaluate and design SVE as a potential component of carbon tetrachloride remediation. This effort can compliment the volatilization research proposed by Vista Engineering. The Vista work is directed towards *surface* behavior of carbon tetrachloride at the disposal sites, whereas our contribution is related to *subsurface* flow and transport phenomena.

Proposed Approach

A targeted set of column and intermediate-scale flow cell experiments and associated model code development is proposed to measure the transfer parameters of kinetic mass associated with the SVE process and to incorporate these parameters into the model code. Experiments will be conducted in the Environmental Molecular Sciences Laboratory's Subsurface Flow and Transport Experimental Laboratory. The experimental studies, based previous SVE experiments, will use contaminant mixtures representative of the mixed organic waste disposed at the 216-Z-9, 216-Z-1A, and 216-Z18 sites (e.g., carbon tetrachloride mixed with poly-butyl phosphates and lard oil) and Hanford Site porous materials. Experimental variables in the column studies are air injection rates, porous media type, moisture content, and non-aqueous phase liquid saturation. The flow cell studies will be used to investigate effects of heterogeneity and non-aqueous phase liquid type (residual vs. free). The STOMP simulator will be modified to account for rate-limited (kinetic) interfacial mass transfer incorporating the parameters measured in the initial laboratory tests. A final two-dimensional experiment will be conducted to obtain an independent data set for testing and verifying the modified simulator for SVE applications.

Schedule, Budget, and Deliverable

The proposed project can be completed within a period of two years to provide an updated kinetic-based model for SVE. A formal Pacific Northwest National Laboratory (PNNL) report describing the laboratory tests, model parameters, and updated STOMP model will be provided as a deliverable.

The budgetary estimate for this proposed work is $240K.