Use of Contaminant Phase Distribution Calculations to Support Compartment-Based Conceptual Site Models

Kurt D. Pennell (kurt.pennell@brown.edu) (Brown University, Providence, RI, USA)
Naji N. Akladiss (naji.n.akladiss@maine.gov) (Maine Department of Environmental Protection, Augusta, ME, USA)

Background/Objectives. The management and remediation of contaminated sites is typically based on a conceptual site model (CSM) that, ideally, accounts for site hydrogeologic conditions, physical and chemical properties of the contaminant(s), relevant attenuation mechanisms (e.g., sorption-desorption, oxidation-reduction), and mass transport processes (e.g., advection, diffusion, dissolution). In practice, most CSMs are based on low resolution aqueous and solid phase data collected using standard subsurface characterization techniques such as soil boring, drive-point sampling, and monitoring wells, which often provide only a minimal understanding of relevant attenuation and transport processes. In an effort to address some of these concerns, in particular, contaminant mass transfer between low- and high-permeability media (i.e., “back diffusion”), compartment-based models were proposed. However, if the contaminant mass is assigned to the different phase compartments (i.e., vapor, NAPL, aqueous, solid phases) based on “aqueous equivalents” or limited site knowledge, inaccurate conclusions could be reached regarding the relative importance of mass transfer processes between phases and media types, which could impact decisions regarding site management and remedy selection. Thus, the objective of this work was to develop a user-friendly contaminant phase distribution tool that can be used by site managers and practitioners to estimate contaminant mass based on soil and chemical properties.

Approach/Activities. Using chemical properties (e.g., aqueous solubility, vapor pressure) and site-specific solid phase data (e.g., organic carbon content, water content) an Excel-based contaminant phase distribution (CPD) spreadsheet was developed to calculate the equilibrium distribution of contaminant mass between the aqueous phase (groundwater), solid phase (soil or aquifer material), gas phase, and free product or organic liquid phase (NAPL). The spreadsheet is designed to use soil boring concentration data, expressed as mg of contaminant per kg of dry soil (mg/kg or ppm), collected from different depths and locations at the field site. The resulting contaminant mass existing in different media types (low permeability, transmissive), phases (vapor, NAPL, aqueous, solid), and site regions (source, plume) can then be implemented into the 14-compartment model framework.

Results/Lessons Learned. The contaminant phase distribution model was used to calculate the equilibrium distribution of trichloroethene (TCE) mass in the source zone and plume region of a site at early (i.e., 5.0% NAPL), middle (1.0% NAPL), and late (0.02% NAPL in source) stages. The mass calculated in each phase was delineated into three categories (LOW < 10% Total Mass; MODERATE = 10 to 50% of total mass; HIGH > 50% Total Mass), and compared to 14-compartment model mass distributions based on “aqueous equivalents”. This analysis showed that the “aqueous equivalence” approach underestimated the TCE mass attributable to NAPL and overestimated mass in the solid phase at early and middle stages. The model was then applied to a soil boring with a measured concentration of 800 mg/kg tetrachloroethene (PCE), and organic carbon content of 0.04% and a gravimetric water content of 5.0%. The calculated equilibrium distribution of PCE in the core was 66% NAPL, 31% solid phase, 1% aqueous, and 2% vapor phases. The phase distribution model can be readily adapted to incorporate non-linear sorption and mixed NAPLs.