Modelling the Recovery of Volatile Organic Compounds during In Situ Thermal Remediation

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Background/Objectives. Soil and groundwater contaminated by non-aqueous phase liquids (NAPLs) can potentially be treated using in situ thermal treatment (ISTT) technologies, including electrical resistance heating (ERH) and thermal conductive heating (TCH). These technologies increase the temperature of the subsurface to create a gas phase composed of steam and vapor, which is subsequently captured, extracted, and treated above ground surface. While many ISTT applications focus on increasing subsurface temperatures, their success relies on the production, capture and extraction of the gas phase; failure to capture gases produced by boiling groundwater and NAPL will result in incomplete NAPL mass removal and possible redistribution of contamination. While numerical models can be useful tools for the design and assessment of ISTT applications, there are few models available that incorporate gas production and flow. Including gas-based processes in ISTT models will allow an investigation of gas-phase mass recovery and its relationship to site conditions (e.g., geology, NAPL distribution), as well as an assessment of potential strategies to improve performance monitoring to reduce both energy and operation time.

Approach/Activities. To investigate the influence of different field conditions on the performance of ISTT, a 2-D finite-difference numerical model was developed to simulate VOC mass recovery during thermal treatment by TCH. This model incorporates conductive heat transport, NAPL-water co-boiling, water boiling, gas migration in the saturated zone, and passive gas extraction. Heat transport is simulated using a continuum approach and gas migration is simulated using a macroscopic invasion percolation (MIP) approach. A spatially-correlated random permeability field was used to generate representative geological realizations, with local correlations to capillary entry pressure. The vapor pressures of water and NAPL were used to determine spatially-variable co-boiling temperatures as a function of depth and capillary entry pressure, and the enthalpy of vaporization of the substances were used to couple phase change with heat transport, with thermal conductivity as a function of gas saturation. The model was applied to multiple realizations of a trichloroethene (TCE) DNAPL release in a 20 m × 5 m domain. Model output included local subsurface temperature, gas saturations and NAPL saturations, as well as VOC mass removal at individual extraction locations.

Results/Lessons Learned. Results from a range of simulated scenarios (multiple realizations for different geology) will be presented to evaluate the impact of soil heterogeneities and NAPL architecture on VOC mass removal rate during TCH treatment. Relationships between local temperature measurements, local mass recovery and overall NAPL removal will be examined to determine the extent to which local measurements can act as an indicator of treatment completion to limit operation time. Simulation results will also be used to investigate cumulative and instantaneous mass recovery curves for various site conditions as a means to infer site conditions and inform decision making during operation.