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MODELLING THERMAL REMEDIATION OF MIXTURES OF VOLATILE AND NONVOLATILE ORGANIC COMPOUNDS

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Summary. Hazardous organic chemicals often exist in the subsurface as mixtures of volatile, semivolatile, and nonvolatile compounds. Several laboratory, field, and modelling studies have shown the promise of thermal remediation methods, such as steam flushing, for the removal of volatile organics. As the volatility of the organic decreases the potential rates of removal decrease. Compounds such as DDT and a number of polyaromatic hydrocarbons which are solid at ambient temperature, are often dissolved in dense nonaqueous phase liquids (DNAPL), and comprise a fraction of the DNAPL that is essentially nonvolatile at typical steam flushing temperatures. Therefore, these nonvolatile compounds, can only be removed in any significant amount by hydraulic displacement of the DNAPL. Many nonvolatiles have melting points such that they are liquid at steam flushing temperatures, making hydraulic displacement feasible even after stripping of the volatiles. However, steam stripping of the volatiles decreases the DNAPL viscosity, reducing the potential hydraulic displacement rates. Downward movement of the melted nonvolatiles into capillary barriers can still be of concern, due to desaturation of the capillary barriers from water vaporization. The presence of the nonvolatile in the DNAPL also produces significant tailing in the removal of the volatiles, as their effective vapor pressures and volatilization rates decrease with preferential removal from the DNAPL.

A three-dimensional finite difference model for three-phase (water-gas-NAPL) flow and transport with energy transport and fully temperature dependent fluid properties and interphase partitioning has been developed and applied to examine the dynamics of removal of mixtures of volatile and nonvolatile organic compounds by steam flushing. The predictions show good agreement with laboratory experiments, and modeling field scale scenarios confirms the challenges in application of steam flushing to remediation of mixtures of volatile and nonvolatile organics. The study also illustrates that modeling the rapid phase changes associated with steam flushing is computationally challenging.