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Relative velocities of DNAPL and aqueous phase plume migration

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Abstract

Numerical simulation is used to examine the relative velocities of DNAPL and aqueous phase plumes in sandy aquifers where lateral spreading of DNAPL has occurred at the base of the aquifer. The scenario being modeled is one where a permeable aquifer is underlain by a sloping aquitard, which results in lateral migration of the DNAPL down the slope, in addition to lateral migration of an aqueous phase plume subject to a specified hydraulic gradient. A sensitivity analysis is presented to the impacts of both DNAPL properties and geologic properties. The most important chemical properties governing the relative velocities of the DNAPL and the shallow aqueous phase plume are the DNAPL viscosity and the aqueous component soil–water partition coefficient (K_d). The dip of the underlying aquitard was found to be relatively unimportant, at least for the range of values studied. The scenario under consideration can be important in conceptual model development and remedial design, as in certain cases DNAPL could be migrating in areas without the evidence of a well-developed aqueous phase plume. The implication of this work is that the absence of a shallow aqueous phase plume directly downgradient of a DNAPL source zone does not rule out the possibility of deep occurrences of DNAPL beyond the shallow monitoring well network. A further finding of this study is that the occurrence of a highly sorbing compound in groundwater at virtually any concentration may indicate the immediate upgradient presence of residual or pooled DNAPL.

Keywords: DNAPL; Velocity; Trichloroethylene; Polychlorinated biphenyl; Creosote; Groundwater

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1. Introduction

Many hazardous compounds commonly found in the subsurface are slightly soluble, highly volatile fluids that are immiscible with water. Despite their low aqueous solubility, these fluids pose a widespread potential threat to groundwater resources. Denser-than-water immiscible contaminants include halogenated hydrocarbons such as trichloroethylene (TCE) and related chlorinated hydrocarbons, polychlorinated biphenyls (PCBs), coal tar and creosote. Collectively, these compounds are referred to as dense, non-aqueous phase liquids (DNAPLs). Considerable effort is underway to understand the migration and distribution of DNAPLs in the subsurface, and to develop methodologies for predicting and controlling their movement and removal.

The rate of DNAPL migration through saturated porous media is governed by capillary, viscous and density effects. The rate of aqueous phase plume migration is typically governed by advection, dispersion, sorption, diffusion and possible degradation effects. Depending on specific fluid and media properties, it is possible that the velocity of the leading edge of a migrating DNAPL body may be coincident with that of the aqueous phase plume derived from dissolution of the DNAPL. Reynolds and Kueper (2001), for example, demonstrated that the vertical migration of chlorinated solvent DNAPL can be coincident with the leading edge of the aqueous phase plume in fractured clay–sand sequences because of the attenuating influence of matrix diffusion. It is also well recognized that the leading edge of an aqueous phase PCB plume, for example, is typically not very far removed from the DNAPL source because of the large degree of sorption exhibited by these compounds.

Understanding the relative velocities of DNAPL and aqueous phase plume migration is important when designing site characterization programs, developing conceptual models and implementing remediation programs. The combination of currently migrating DNAPL and a highly retarded plume, for example, could lead to inappropriate placement of pump-and-treat extraction wells and passive barriers. Observing an aqueous phase breakthrough curve in a deep monitoring well in a situation where the DNAPL and plume velocities are coincident, for example, would indicate DNAPL presence at that location. It is important that conceptual models distinguish between cases where the velocities of the DNAPL and aqueous phase plumes are similar, and cases where they are not.

The objective of this study is to utilize numerical simulation to systematically investigate the fundamental parameters governing the relative velocities of migrating DNAPL and aqueous phase plumes in sandy aquifers. Simulations are carried out investigating the migration of TCE, PCB and creosote DNAPLs along with representative aqueous phase components.

2. Multiphase flow and transport model

This study utilizes a three-dimensional, multiphase compositional finite volume model (QUMPFS) that simulates the fate and transport of both dissolved and NAPL substances (Reynolds and Kueper, 2001). The QUMPFS model is based on the partial differential equations governing isothermal multiphase flow with multi-component transport in porous media. The model has the ability to simulate multiphase, advective, dispersive and diffusive flux of NAPL constituents in porous media. Additional features include capillary pressure hysteresis based on Gerhard et al. (1998), the formation of non-wetting phase residual based upon saturation history, equilibrium and nonequilibrium mass transfer of constituents between phases, and a flux limiting scheme to control numerical dispersion. Full details of the model and its underlying numerical foundation can be found in Reynolds and Kueper (2001).