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An analytical model for predicting LNAPL distribution and recovery from multi-layered soils

Jaehak Jeong [a,*], Randall J. Charbeneau [b,1]

[a] Texas A&M AgriLife Research, Texas A&M University System, Temple, TX, United States
[b] Department of Civil, Architectural, and Environmental Engineering, University of Texas at Austin, Austin, TX, United States

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ABSTRACT

An analytical model was developed for estimating the distribution and recovery of light nonaqueous phase liquids (LNAPL) in heterogeneous aquifers. Various scenarios of LNAPL recovery may be simulated using LDRM for LNAPL recovery systems such as skimmer wells, water-enhanced wells, air-enhanced wells, and trenches from heterogeneous aquifers. LDRM uses multiple horizontal soil layers to model a heterogeneous aquifer. Up to three soil layers may be configured with unique soil properties for each layer. Simulation results suggest that LNAPL distribution and its recovery volume are highly affected by soil properties. In sandy soils LNAPL can be highly mobile and the recovery efficiency can be high. In contrast, even at high LNAPL saturations, LNAPL mobility is typically low in fine-grained soils. This characteristic of LNAPL with respect to soil texture has to be carefully accounted for in the model to better predict the recovery of LNAPL from heterogeneous soils. The impact of vertical hydraulic gradient in fine grain zone was assessed. A sensitivity analysis suggests that the formation LNAPL volume can be significantly affected by a downward vertical hydraulic gradient if the magnitude is near a critical amount ($=\rho_r - 1$). Sensitivity of input parameters with respect to LNAPL formation in soils and LNAPL recovery volume were identified through a sensitivity analysis. The performance of LDRM on predicting the distribution and recovery of LNAP was reasonably accurate for a short-term analysis as demonstrated in a case study. However, further validation is needed to ascertain the model's performance in long-term simulations.

1. Introduction

Nonaqueous phase liquids (NAPLs) are contaminants that exist as a separate immiscible phase in the subsurface. NAPLs include petroleum products such as gasoline and oils, and solvents such as trichloroethylene (TCE). Light nonaqueous phase liquids (LNAPLs) are lighter than water and are either immiscible or only partially miscible in water. When there is a LNAPL release into the soil, it migrates downward through the subsurface under the influence of gravity until it reaches the water table, where it forms a LNAPL lens and spreads laterally. As the LNAPL spreads, some of it may be left behind as residuals and other volatile constituents may move into the subsurface vapor phase and spread in the vadose zone. Soluble constituents from the LNAPL lens may dissolve into the groundwater flowing beneath the lens, forming a contaminated groundwater plume.

Many LNAPL recovery systems in operation employ either single- or dual-pump recovery wells. However, only limited guidance is currently available regarding how best these systems can be operated for the optimum long-term LNAPL recovery (Charbeneau et al., 1999). To address the application of proven technologies for recovering LNAPL releases to groundwater, the API developed a set of spreadsheet models that calculate the distribution and recovery of LNAPL from soils using conventional recovery technologies (Charbeneau,

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* Corresponding author. Tel.: +1 254 774 6118.
E-mail addresses: jjeong@brc.tamus.edu (J. Jeong), Charbeneau@mail.utexas.edu (R.J. Charbeneau).
[1] Tel.: +1 512 471 0070.

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2003; Charbeneau et al., 1999). These models have not only been recommended by agencies (US Army Corps of Engineers, 1999; US EPA, 2005), but also been used in numerous scholastic researches (Adamski et al., 2005; Huntley and Beckett, 2002; Johns et al., 2003; Li and Yang, 2005; Prakash, 2005; Sleep et al., 2000). LDRM is essentially an upgrade of the earlier spreadsheet models which were coded using Visual Basic functions formulated for the spreadsheet models.

A fundamental assumption of LDRM is that vertical equilibrium conditions apply so that the formation LNAPL distribution can be determined directly from the elevation of air/LNAPL and LNAPL/water interfaces measured in monitoring wells (Farr et al., 1990; Lenhard and Parker, 1990). LNAPL distribution and mobilization is represented using the capillary pressure–saturation–permeability models proposed by van Genuchten (1980), Mualem (1976), and Burdine (1953). Vertical distributions of hydrocarbon saturation and relative permeability are calculated based on the assumption of vertical equilibrium. In a three-phase system of air, water, and LNAPL, there is no direct contact of water by air, so the air and LNAPL capillary pressure is a function of the total liquid saturation. The capillary pressure between the LNAPL and water phase is a function of the water saturation where water is the wetting fluid (Leverett, 1941; Parker et al., 1987).

Understanding the groundwater hydraulics and contaminant transport in heterogeneous soils is a great challenge because of the highly preferential flows promoted by physio-chemical properties of the soils (Kelly and Pomes, 1998). For example, clay-pan is a thin layer in the subsoil that promotes preferential flows with much greater clay content than over- and under-lying soils, which is prevalent in regions of the mid-west United States including Illinois, Indiana, Kansas, Missouri, Ohio, and Oklahoma (Jamison et al., 1968). In fine grain soils where macropores might exist, a vertical migration of LNAPL far below groundwater table has been observed in several areas in the U.S. (Adamski et al., 2005). To address this issue, an algorithm for assessing the impact of the vertical hydraulic gradient was developed and added to LDRM.

The objective this paper is to develop algorithms that describe the vertical distribution of LNAPL, its lateral transport in the vadose zone, and the removal rate based on the pressure gradient caused by conventional removal technology such as air injection or water injection and pumping. The significance of input parameters is investigated with respect to various types of LNAPL, soil types, and recovery technologies in a sensitivity analysis. The performance of the model is evaluated in a case study in which LDRM is used to simulate LNAPL distribution and recovery prediction from pumping wells at a LNAPL spill site (formerly a U.S. refinery).

2. Methods

2.1. LNAPL vertical saturation distribution

The relationship between fluid saturation and capillary pressure is defined by van Genuchten (1980) model.

$$S_{we} = \left(\frac{1}{1+(\alpha\Psi)^N}\right)^M \tag{1}$$

where S_{we} is the effective water saturation and Ψ is the capillary pressure head. M, N and α are empirical parameters. The dimensionless exponents M and N are related to pore size distribution and relate to each other by $M = 1 - 1 / N$ for the Mualem relative permeability model ($N > 1$) and $M = 1 - 2 / N$ for the Burdine relative permeability model ($N > 2$). α is related to the fluid interfacial properties and effective pore size. Generally, α and M are larger for coarse, well-sorted soil. The effective water saturation is scaled such that it ranges from zero (dry soil with water at residual water saturation) to one (fully saturated).

Under the assumption of vertical equilibrium, Eq. (1) may be associated with capillary pressure relations to describe the vertical saturation distribution of LNAPL and water in a three-phase system. Using the Leverett assumptions (Charbeneau, 2007) for the LNAPL-water pair, the water saturation distribution in stratified soil layers can be represented by the following equation.

$$S_w(z) = S_{wr,i} + \left(1 - S_{wr,i} - S_{nr,i}\right)\left(\frac{1}{1+\left(\alpha_{nw,i}(z-z_{nw})\right)^{N_i}}\right)^{M_i} \quad i = 1, 2, or\, 3 \tag{2}$$

where $S_{wr,i}$ is residual water saturation in soil layer i, $S_{nr,i}$ is residual LNAPL saturation (non-recoverable) in soil layer i, α_{nw} is the scaling parameter for the capillary pressure between LNAPL and water, and z_{nw} is the elevation of LNAPL/water interface in the monitoring well. Water saturation is defined as a function of the LNAPL and water capillary pressure, while the total liquid saturation (including water and LNAPL) is a function of the air and LNAPL capillary pressure.

$$S_t(z) = S_{wr,i} + S_{nr,i} + \left(1 - S_{wr,i} - S_{nr,i}\right)\left(\frac{1}{1+\left(\alpha_{an,i}(z-z_{an})\right)^{N_i}}\right)^{M_i} \tag{3}$$

$i = 1, 2, or\, 3$

In Eq. (3), z_{an} is the elevations of air/NAPL interface in the monitoring well. Once $S_w(z)$ is known, LNAPL saturation is computed by $S_n(z) = S_t(z) - S_w(z)$.

The amount of hydrocarbon present in the polluted subsurface soils can be estimated by integrating the LNAPL saturation over the interval of continuous LNAPL region. The specific LNAPL volume (D_n), defined as the volume of LNAPL per unit surface area is calculated from Lenhard and Parker (1990):

$$D_n = n \int_{z_{nw}}^{z_{\max}} S_n(z) dz \tag{4}$$

In Eq. (4), n represents the porosity of porous medium, z_{max} is the highest elevation of free LNAPL due to capillary rise corresponding to a specified monitoring well LNAPL thickness, and z_{nw} is the elevation of the LNAPL/water interface. LNAPL is considered mobile when the saturation is larger than residual amount. The residual LNAPL cannot be recovered by liquid recovery technologies. Therefore, the recoverable LNAPL specific volume corresponds to the area