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Simulations of LNAPL flow and distribution in heterogeneous porous media under dynamic hydrogeologic conditions

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ABSTRACT

불포화대에서 LNAPL의 이동과 분포를 수치 모의를 통하여 예측하였다. 균질한 매질에서 LNAPL의 이동은 조립질 매질에서 빠르고, 세립질 매질에서 더 많은 면적으로 확산되며, 더 많은 LNAPL이 불포화대에 잔류한다. 조립질 매질내에 세립질층이 존재할 경우, 이 층이 지하수면으로부터 멀수록 LNAPL이 많이 포획된다. 조립질 매질에 세립질 또는 더 조립질인 매질이 렌즈 상으로 존재하는 환경에서는, LNAPL이 이들 렌즈를 통과하지 못한다. 불균질한 렌즈가 존재할 때의 LNAPL 분포를 초기조건으로 이용하여, 지하수 면의 수직 이동과 물의 침투에 따른 LNAPL의 이동을 모의하였다. 두 경우 모두 불포화대에 잔류되어 있던 LNAPL의 수직방향 이동이 증가되었다. 특히, 지하수면의 하강 시 LNAPL이 조립질 렌즈를 통해 이동하나, 세립질 렌즈를 통해서는 이동하지 못한다.

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key word : LNAPL, Multiphase flow, Numerical simulation, Capillary barrier

I. Introduction

The contamination of soil and ground water by nonaqueous phase liquids (NAPLs) has become a major environmental problem. Because NAPLs are immiscible fluids, if NAPLs are spilled in the subsurface, they migrate under the influence of capillary, gravity, and buoyancy forces as separate free phases. Especially, LNAPLs are less dense than water. They can percolate unsaturated zone and be accumulated on the water table. If enough amount of LNAPLs is introduced into the subsurface, it spreads out on top of water table and contaminates a significant volume of soil and ground water. Because improved knowledge on flow and distribution mechanisms of LNAPLs in the subsurface is required for risk assessment and remediation design, it is important to understand the behaviors of LNAPLs in the subsurface.

To understand the behaviors of LNAPLs in the subsurface, numerical modeling (Kaluarachchi and Parker, 1989) and physical modeling (Schroth et al., 1998) have been performed. According to the previous researches, the behaviors of LNAPLs are generally dependent on subsurface heterogeneity, its geometry and hydrologic conditions. But the understanding of LNAPL flow and distribution mechanisms in heterogeneous unsaturated zone is still incomplete. LNAPL behaviors under dynamic hydrologic conditions such as water table fluctuation and rainwater infiltration are not also fully understood.

The objective of this research is to examine how LNAPL flow and distribution are influenced by subsurface heterogeneity, water table fluctuation and rainwater infiltration through numerical simulations. Numerical simulations were performed using the Subsurface Transport over Multiple Phase (STOMP) simulator.

II. STOMP simulator

STOMP is a three-dimenstional, three-fluid compositional simulator for modeling contaminant flow and transport in variably saturated porous media (White and Oostrom, 1996). Simulations in this research were conducted with water-oil mode, which solves isothermal problems involving the simultaneous flow of an aqueous phase and an NAPL with passive gas phase. The governing equations are discretized using the intergrand -volume finite difference method with fully implicit time differencing, and are solved with a Newton-Raphson iteration method. As the relative permeability-saturation -capillary pressure (k-S-P) relations, entrapment van Genuchten (Parker and Lenhard, 1987)/Mualem (Mualem, 1976) model was used.

III. Numerical simulations

The numerical experiments consist of numerical tests simulating NAPL spill and distribution in unsaturated, two-dimensional domain (10m×5m). Five different porous materials were used in the simulations. Toluene as a LNAPL was selected.

1. Homogeneous case (case 1)

Sand and silt loam were chosen as homogeneous porous materials to examine the difference of LNAPL flow and distribution in homogeneous fine and coarse material. During simulations, the water table was maintained at 3.5m below the top surface. The release of LNAPL at 1m strip in the middle of top surface was applied using time-dependent Neumann boundary conditions during 66 days.

The LNAPL infiltrated more rapidly in the sand. But the evolution of the LNAPL front followed similar patterns in both materials. The LNAPL front advanced with a circular shape in the unsaturated zone. When the front arrived at the water table, the spreading in the unsaturated zone came to halt, and the bulk of LNAPL was contained within a pancake-shaped lens situated on top of the water table. The contaminated soil volume was slightly larger, more LNAPL retained in silt loam, and the thickness of pancake-shape lens was slightly larger in the silt loam.

2. Heterogeneous case with layer (case 2 : silt loam layer in sand)

To investigate LNAPL flow and distribution in coarse materials with a fine layer, LNAPL was injected in sand with silt loam layer. In this simulation, the silt loam layer was 0.4 m thick and the location was changed three times; upper, middle, and lower part in the unsaturated zone. The simulation domain, initial and boundary conditions were same for case 1. The initial pattern of LNAPL flow was similar with that of the homogeneous material. However, slightly lateral movement took place along layer boundaries (Figure 1) and more LNAPL was retained when the layer was located at upper part of the unsaturated zone. Although the contaminated soil volume was not different for three cases, the retained volume of LNAPL in the unsaturated zone was largest when silt loam layer was situated at upper part in the unsaturated zone.

3. Heterogeneous case with lens (case 3-1 : silty clay loam or gravel lens in sand)

To evaluate LNAPL flow and distribution in coarse sand with fine sand lens and coarser sand lens, LNAPL evolution was simulated in sand containing isolated lens of either silty clay loam or gravel. The results show LNAPL diverted around both the silty clay loam lens and gravel lens (Figure 2). The diversion on top of silty clay loam lens is owing to the low permeability of this lens. But the diversion on top of gravel lens is a result of the capillary barrier effect between the gravel and the sand.

4. Water table fluctuation (case 3-2)

Fluctuation of water table was simulated to investigate behaviors of LNAPL retained in case 3-1 under a water table fluctuation condition. In both silty clay loam lens and gravel lens, LNAPL flow was enhanced in the down direction by water table fluctuation. When water table was raised, LNAPL was accumulated on the rising water table. But LNAPL behaviors were different in both cases with water table lowering. While in case of gravel lens most of LNAPL passed through the gravel lens (Figure 3), large amount of LNAPL diverted silty clay loam lens and pass through the sand.

5. Rainwater infiltration (case3-3)

LNAPL infiltration under static water table conditions (case 3-1) was followed by infiltration of water to examine the effect of rainwater infiltration to LNAPL distribution. Percolation of LNAPL retained in the sand above heterogeneous lens was enhanced in both silty clay loam and gravel lenses. At early stage, more amount of LNAPL was retained on top of lens than the case without water infiltration. After that, retained LNAPL spreaded on top of lens and moved downward.

IV. Summary and conclusion

The nature of LNAPL movement in the subsurface was investigated through numerical simulations. In case of homogeneous media, the vertical movement is faster in the sand. But the total contaminated area and the volume of LNAPL retained in the vadose zone is larger in the silt loam. When silt loam layer exists in sand, the quantity of LNAPL retained in the vadose zone depends on the location of the layer. Larger amount of LNAPL is retained as the layer is situated in the upper part. LNAPL percolation in the sand with heterogeneous lens, where the unsaturated material properties are very different from sand, shows that the contrasting material properties have significant effects on LNAPL flow and distribution within the unsaturated zone. Under the condition of water table fluctuation and rainwater infiltration, LNAPL percolation is increased. In case of gravel lens, most of LNAPL, retained on top of the lens, passed the gravel lens when the water table is lowered. The LNAPL flow and distribution observed in this numerical experiments show the behaviors of LNAPL in the subsurface highly depend on heterogeneous unsaturated environment and the dynamic hydrologeologic conditions such as water table fluctuation and water infiltration. These results can explain some of the complexity of LNAPL flow and distribution patterns in LNAPL contaminated field sites.

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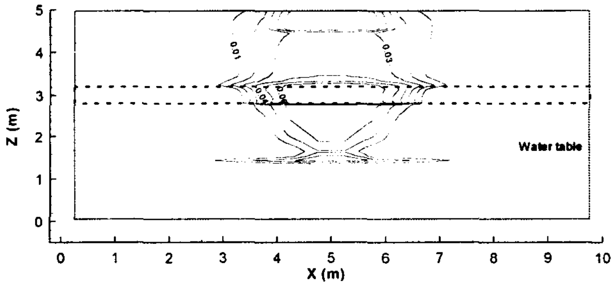

Figure 1. Simulated LNAPL content at t=120 days when silt loam layer exist in sand. The dashed rectangle is silt loam layer.

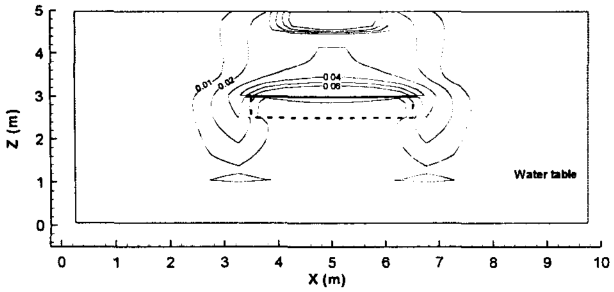

Figure 2. Simulated LNAPL content at t=80 days when gravel lens exist in sand. The dashed rectangle is gravel lens.

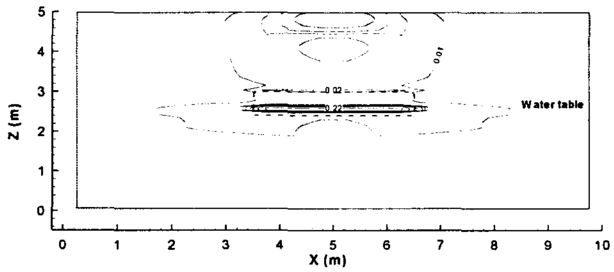

Figure 3. Simulated LNAPL content at t=8 days after water table fluctuation when gravel lens exist in sand. The dashed rectangle is gravel lens.