SIMULATION OF DNAPL DISTRIBUTION RESULTING FROM MULTIPLE SOURCES

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ABSTRACT: A three-dimensional and three-phase (water, NAPL and gas) numerical simulator, called NAPL, was employed to study the interaction between DNAPL (PCE) plumes in a variably saturated porous media. Several model verification tests have been performed, including a series of 2-D laboratory experiments involving the migration of PCE through a variably saturated, homogeneous sand. A comparison of the experimental data to the model results illustrates the effect and importance of fluid entrapment and saturation hysteresis.

The NAPL model was used to simulate a 3-D multi point PCE source release within a contained test cell at the Groundwater Remediation Field Laboratory (GRFL) in Dover, Delaware. In this experiment, the migration of PCE in the unsaturated and saturated zones, under various infiltration scenarios, was simulated. The modeling of multiple injection points in a homogeneous aquifer shows that the ultimate distribution of PCE depends on the injection point locations and the time-varying release rates, and the depth to the water table. In general, an intermittent, slow, injection rate caused narrow, deeply penetrating DNAPL plumes. On the other hand, higher injection rates resulted in a wider horizontal distribution and more interaction between neighboring plumes, thus creating non-symmetric distributions and an increase in the flow rate and depth of penetration.

INTRODUCTION

A 3-D NAPL model was developed to investigate the movement of organic compounds in both homogeneous and heterogeneous porous media. Particular attention was paid to the development of a sub-model that describes three-phase hysteretic permeability-saturation-pressure relationships, and the potential entrapment of fluids when they are displaced. Several laboratory experimental data sets have been compared to simulator predictions, including a series of 2-D laboratory experiments involving PCE release conducted by the authors at the R. S. Kerr Laboratory, Ada OK, and described in Fishman et al. (1998) and Guarnaccia et al. (1997).

The results of modeling runs were used to develop a DNAPL release strategy for remediation technology demonstrations at the Dover National Test Site (DNTS), Dover, Delaver, and to predict the DNAPL movement from injection points under a range of hydrodynamic release conditions. Because the hydrodynamic properties and spatial variability of these properties strongly influences the behavior of DNAPL in the subsurface, simulations were done for a range of hydrodynamic conditions in both homogeneous and heterogeneous porous media.

The attributes (parameters, processes) that control DNAPL distribution in subsurface granular porous media include: fluid properties (density, viscosity, interfacial tension, wettability), soil properties (hydraulic conductivity, heterogeneity), source conditions (release rate and proximity of multiple sources). The focus of this paper is on the issue of source conditions: how release rates and source proximity affect DNAPL distribution in the subsurface.

NUMERICAL MODEL

A numerical model, called NAPL (Guarnaccia et al., 1997), was used to simulate the experiment described above. The model has the following conceptual and computational attributes, which are assumed to be relevant to the physical experiment to be modeled:

1. simultaneous flow of water, NAPL, and gas;
2. the three-phase relative permeability-saturation-capillary pressure (k-S-P) relationships are based on fluid phase wettablility considerations and two-phase data; wettability follows, from most to least, water-NAPL-gas;
3. the three-phase k-S-P model reduces to the appropriate two-phase model when appropriate;
4. the k-S-P model includes flow-path-history-dependent functionals (hysteresis);
5. the k-S-P model includes a mechanism for fluid entrapment during drainage (residual emplacement), where the amount entrapped is a function of the maximum imbibed saturation;
6. the S-P model employs capillary pressure scaling to account for variable porous medium and fluid properties;
7. at each boundary node, one can specify either a no flow condition (can also be coupled with a point source or sink 'well' rate for one or more phases), or any one of the three phase pressures known, or all the primary variables known (i.e., one pressure and two saturations);
8. a numerical 'peclet criterion' can be employed to ensure that the scale of the saturation–capillary pressure functional is compatible to the scale of the grid.

The model employs the collocation finite element method to approximate the system of governing equations spatially, and an implicit finite difference approximation in time. The non-linear system of governing equations is solved using a sequential solution algorithm. Details of the numerical methods can be found in Guarnaccia et al. (1997).

NUMERICAL EXPERIMENTS

Model Testing. A two-dimensional artificial aquifer experiment was conducted to study how DNAPL (PCE) migrates through a variably saturated homogeneous, isotropic, porous medium. A video image of the experiment was analyzed to define the DNAPL saturation at the pixel-scale as a function of time. Once constructed, the image was compared to the solution of the numerical model designed to simulate the same experiment. When the image was averaged to the same spatial scale as the model grid, a qualitatively similar solution was observed.

Figure 1 compares the image of experimental distribution of PCE and the numerical results at T = 60min (as the PCE is migrating through the saturated zone). Note that the solutions are qualitatively similar, indicating that the numerical model effectively captures the physics of the problem as defined at the scale of a grid cell. This information can be used in practice to define appropriate dissolution and vaporization mass transfer rates at the grid scale. Details of the experiment and the video imaging analysis can be found in Fishman et al. (1998).

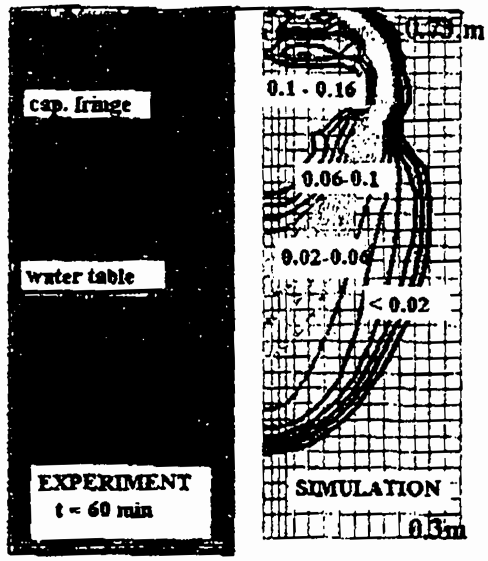

FIGURE 1. Experiment and model simulation.

Effects of Heterogeneity on DNAPL Distribution. It is well known that DNAPL distribution in the subsurface is very sensitive to heterogeneity in hydraulic conductivity (see for example Poulsen and Kueper, 1992, and Kueper et al., 1993). The effect of soil heterogeneity on PCE distribution is illustrated in Figure 2. The same PCE flood experiment was run in a variably saturated domain with three hydraulic conductivity (K) realizations: a homogeneous domain (part a), a horizontal low K lens located below the water table (part b), a vertical high K lens located below the water table (part c). The low K horizontal lens exerts a very strong influence on the PCE migration pattern. The inability to penetrate this lens is due to a combination of preferential flow through high K sand and the fact that the capillary pressure above the lens is less than the entry pressure for the lens (Figure 2 b). Conversely, the high K vertical lens enhances vertical PCE migration via the combination of preferential flow and the low entry pressure associated with the lens (Figure 2 c).

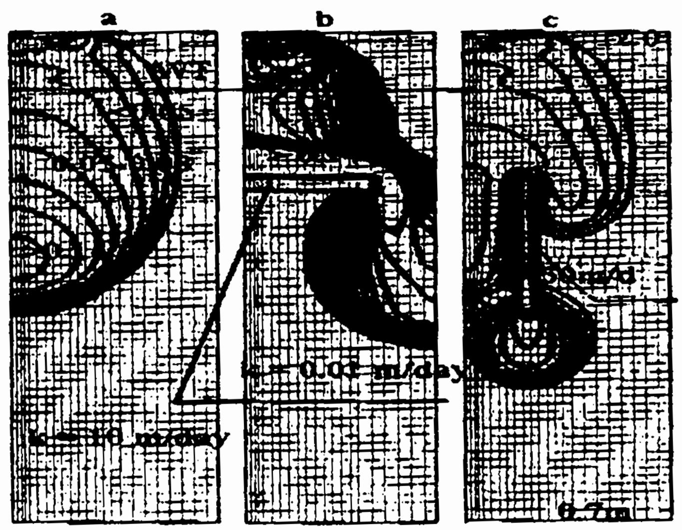

FIGURE 2. PCE saturation distribution. a-homogeneous media. b-single horizontal lense. c- single vertical lense.

The simulations show that heterogeneity causes the shape and internal structure of the DNAPL plume to differ significantly from that predicted using the homogeneous realization. At the field scale, because of uncertainties in defining soil properties, and computational issues regarding discretization, DNAPL modeling becomes one of a sequential screening exercise. Specifically, initial modeling with a mean homogeneous K-field is combined with data generated from a groundwater quality profile located down-gradient of the source (see Pardieck and Guarnaccia, 1999). An appropriate 'modeling K-field' is defined using the groundwater quality profile signature.

Effects of Source Rate, and Multiple Release Locations. In this section we present results of several 3-D PCE flood numerical experiments aimed at providing insight into the importance of source area characterization in assessing DNAPL distribution in the subsurface. Specifically, we consider the variables of source release rate and the number and proximity of sources. The 3-D domain is homogeneous, while the source distribution is heterogeneous.

Soil-and Fluid-Phase Parameters. The model parameters, which are presented in Table 1, were determined in the laboratory or obtained from literature.

TABLE 1. Parameters used in the DNAPL spill simulations.

Soil Properties

porosity - 0.37; hydraulic conductivity - 10 m/day; volume density - 1.7 g/cm^3.
van Genuchten k-S-P parameters: a_d - 4.00/m; a_i - 6.00/m; n-6.35;
DNAPL residual saturation as a nonwetting phase - 0.14.

DNAPL properties

viscosity - 0.90 Cp; density - 1.626 g/ml; interfacial tension, PCE -water- 47.5 dyne/cm; interfacial tension, PCE- air - 31.74 dyne/cm.

Water properties

viscosity - 0.99 Cp; density - 0.99 g/ml; interfacial tension, air-water - 72.75 dyne/cm.

Air properties

viscosity - 0.02 Cp; density - 0.00129 g/ml.

The Flow Domain. The dimensions of the flow domain selected for 3-D multi-well simulations are 200 cm high, 460 cm long, and 300 cm wide. The domain is discretized into an irregular grid of 10 by 26 by 24 elements with spacing that varies from 5.0 by 5.0 by 5.0 cm in proximity to the potential source

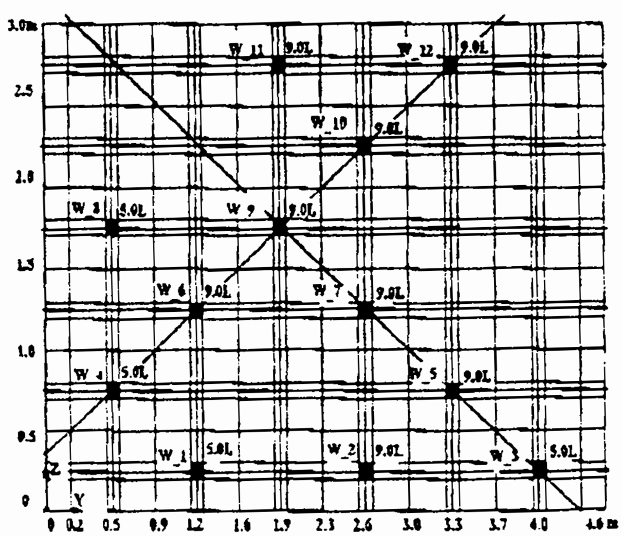

FIGURE 3. Horizontal domain and well locations.

areas to 30.0 by 30.0 by 30.0 cm at the perimeter of the domain. A plan view of the domain is shown in Figure 3 and a cross section is shown in Figure 4.

Initial, Point Source, and Boundary Conditions. The domain is initially free of PCE. PCE flood simulations were performed in which PCE was allowed to infiltrate from as many as twelve point sources located below ground surface, but above the water table, at a rate between 0.25 L/min and 0.9 L/min (total volume injected at any one well ranges from 5.0 to 9.0 L). The locations of the point sources are shown in Figure 3. The boundary conditions are no-flow along all boundaries except the top, where a constant atmospheric pressure is prescribed.

The full experiment was modeled as a sequential series of three sub-models. Each sub-model solves a part of the overall flow problem:
1. The initial conditions for sub-model 1 were full water saturation. At time>0, the water table was lowered between 20 and 40 cm and the two-phase system (water and gas) was allowed to approach steady-state conditions. The final distribution of water saturation was adopted as the initial conditions for second sub-model.
2. Using the initial conditions (distribution of water saturation) determined from sub-model 1, DNAPL was released at a predefined rate from the source(s) until a predetermined total volume was released.
3. After the DNAPL was released to the formation the spill was allowed to redistribute for the duration of the five day simulation period.

For multiple simulations involving changing parameters (e.g., source conditions), this structure allows for restart at known intermediate flow conditions, and thus, it is a time saving measure.

RESULTS AND DISCUSSION

Effect of Injection Rate on DNAPL Distribution. Figure 4 (cross-section) shows the solution after a ten minute release of PCE and five days of redistribution from two point sources: at the source on the left, 5.0L of PCE were injected, while at the source on the right 9.0 L were injected. The results show that as the release rate increases the DNAPL plume tends to spread more laterally. The higher volume injected on the right and resulted in deeper penetration into the saturated zone. For the case of equivalent volume

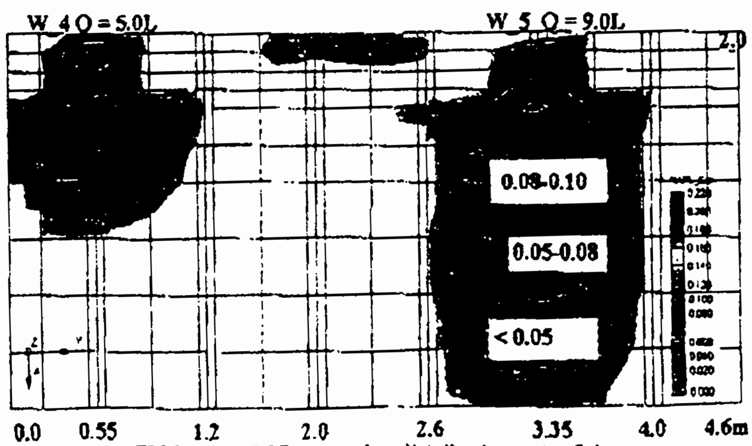

FIGURE 4. PCE saturation distribution at t = 5 days

injected at different rates (not shown), the slower rate resulted in a plume which had a smaller effective radius and greater penetration. This result is consistent with that described in Poulsen and Kueper (1992).

The Multi Wells Simulations. A 3-D simulation was performed in which PCE was allowed to infiltrate from twelve point sources located in the vadose zone (see Figure 3, plan view). Each well injected between 5.0 and 9.0 L of PCE in approximately 10 minutes (the volume for each well is shown in Figure 3). After injection the PCE was allowed to redistribute for five days simulation time.

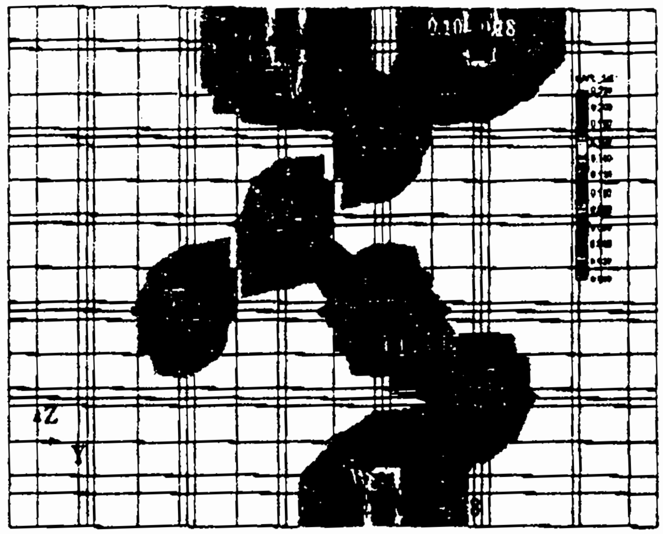

FIGURE 5. Distribution of PCE saturation at depth 200 cm.

Below the water table the extent of the PCE plume reached the bottom and in three areas of PCE release (W_2; W_11 and W_12) it accumulated as a 'pool' of free phase (mobility > 1) (Figures 5 and 6). Pools were created due to the proximity of the wells (20cm) to the impervious walls. In the rest of the area, with a release amount of 9.0 L, the

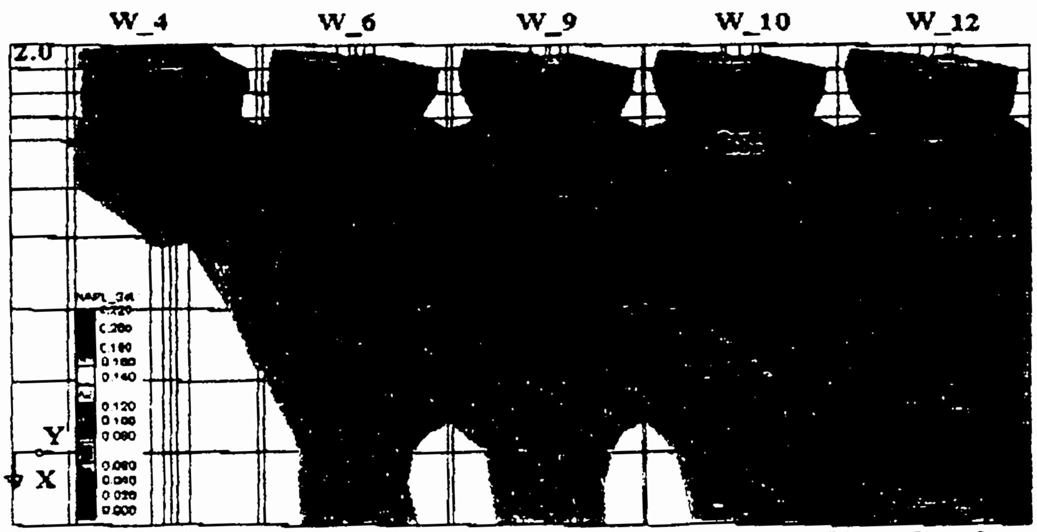

FIGURE 6. Distribution of PCE saturation at cross section W_4 - W_12

plume may reach the bottom but no pool will be created.

Figure 7(a) presents the simulation when distance between wells is 1.0m and less than spreading area (1.4m) shown in part b of Figure 7. In this case we have more interaction between neighboring plumes, thus creating non-symmetric distributions and an increase in the flow rate and depth of penetration. The free phase of DNAPL will accumulate at the bottom of the cell.

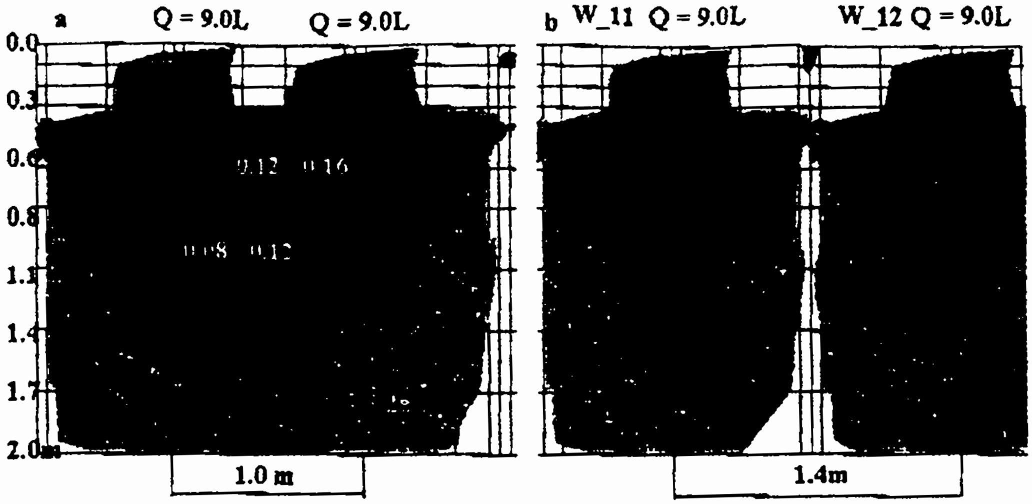

FIGURE 7. PCE saturation distribution.
a - distance between wells is 1.0m. b - distance between wells is 1.4m.

CONCLUSIONS

Three important conclusions have been drawn from the modeling experiments:

a) The depth and the width of spreading PCE are influenced by the release rate and the amount of release. A smaller rate of PCE release gives deeper penetration and a smaller radius of influence than from an instantaneous spill. Our laboratory and modeling experiments confirmed this conclusion;

b) The proximity of multiple sources on DNAPL distribution has an important effect on overall DNAPL distribution, in that coalescence of individual plumes will result in deeper penetration into the saturated zone;

c) Comparison to both laboratory and field DNAPL flood and redistribution experiments indicates that this and other NAPL models are capable of capturing the physics of the problem. However, at the field scale, uncertainty in the most important 'driving' parameters, hydraulic conductivity and source conditions (location and release rate history), as well as, computational issues (discretization limitations), requires that DNAPL modeling be combined with groundwater quality profiling data. The profiling data provides an indication of DNAPL location, and the model is used to obtain a meaningful realization using 'effective' parameters for screening and remediation purposes.

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16. ABSTRACT

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