SENSITIVITY OF CONSTITUTIVE MODELS IN THE PREDICTION OF DNAPL INFILTRATION AND REDISTRIBUTION IN HETEROGENEOUS POROUS MEDIA

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ABSTRACT

Subsurface heterogeneity has a significant influence on infiltration and redistribution of DNAPLs. Even though numerical models may not be able to predict accurately the behavior of DNAPLs in field situations, they can be used to obtain useful insights to design effective remediation schemes. A number of multiphase flow codes with the ability to capture the fundamental processes that control the migration of DNAPLs exist. However, the issue of which constitutive model and parameters need to be used as inputs in these codes to simulate DNAPL infiltration and re-distribution is not studied adequately. With the goal of contributing to the knowledge needed to address this issue, detailed modeling studies were conducted for different representations of retention and imbibition behavior based on two commonly used constitutive models. A series of experiments were conducted to generate an accurate data set on the migration of DNAPLs in synthetic test aquifers with various combinations of heterogeneous/homogenous packing configurations. Model simulations were conducted using a comprehensive multiphase flow simulator, UTCHEM during the injection and redistribution phases of the DNAPL migration. The simulated NAPL infiltration and redistribution using the selected constitutive model representations were compared against with the qualitative data from two sets of experiments. The analysis shows during injection phase, all of the five selected cases of constitutive models were able to match the experimental observations reasonably well with a small time tag. During redistribution, none of the models was able to match the experimentally observed distribution behavior. This preliminary analysis suggests that further detailed study is needed to with more quantitative data to determine which constitutive model and parameters are appropriate to be used in model simulations.

1. INTRODUCTION

Contamination of the subsurface environment by organic industrial chemicals and petroleum derivates such as chlorinated solvents or poly-nuclear aromatic hydrocarbons is a common occurrence. Because of their low solubility, these compounds exist as separate non aqueous phase liquids (NAPLs). Among the organic chemicals, chlorinated solvents that are in the form of dense non aqueous phase liquids (DNAPLs) are frequently encountered at field sites. In order to preserve groundwater resources from contamination and to clean up sites contaminated with these compounds, it is necessary to understand the migration and distribution of DNAPLs in subsurface systems. Fundamental processes that govern the infiltration and redistribution of multiphase fluids are complex, and a considerable research effort is underway to understand these systems more fully. Laboratory and field observations suggest that geologic heterogeneity at different scales has a significant influence on flow and distribution of DNAPLs in the subsurface. As the heterogeneity at all relevant scales cannot be accurately characterized, numerical models may not be able to accurately predict the DNAPL behavior in the field. However, models may be able to predict the general behavior such as possible flow pathways and approximate arrival times. As field data for validation of such models are not available, data generated under controlled conditions in intermediate scale laboratory tanks can be used for this purpose.

Heterogeneity in soil properties contributes to complex entrapment distribution of DNAPs in the subsurface (Schwille, 1988; Kueper et al., 1989; Illangasekare et al., 1995, Essaid and Hess, 1993; Illangasekare et al., 1998; Dekker and Abriola, 2000a). A number of DNAPL experiments conducted in the laboratory (Schwille, 1988; Kueper et al., 1989; Illangasekare et al., 1995; Oostrom et al., 1999) and in the field (Kueper et al., 1993; Brewster et al., 1995) have shown the influence of fluid and soil properties on the infiltration and distribution of DNAPLs. Kueper and Frind (1991) validated a two-phase flow model under simple two dimensional heterogeneous conditions for drainage. Modeling studies have indicated that hysteresis and entrapment must be included in numerical models to simulate accurate infiltration and redistribution of NAPLs in the subsurface (Essaid et al., 1993; Kueper et al., 1993; Van Geel and Sykes, 1994). Gerhard and Kueper (2003a & 2003b) developed a new constitutive model and validated it against using experimental data generated in column studies. Gerhard and Kueper, (2003) conducted numerical simulations to study the influence of constitutive model parameters on DNAPL infiltration and distribution in heterogeneous media at the field scale. They reported that none of the simple (Brooks and Corey and van Genuchten) or more conventional constitutive models were able to reproduce ±10% variations of DNAPL migration between the models, especially during the redistribution.

Many constitutive models have been used in multiphase flow simulations in field and laboratory settings (Burdine, 1953; Mualem, 1976; Brooks and Corey, 1964; van Genuchten, 1980; Lenhard and Parker, 1987; Gerhard and Kueper, 2003a and 2003b). However, none of these models have been adequately validated for their ability to predict DNAPL infiltration and distribution under variety of conditions encountered in the field. Available laboratory data is limited to simple packing configurations (e.g. lenses, horizontal, layers). These test configurations do not realistically represent or capture all the geologic complexities of field systems (e.g. inclined layers, stratifications, embedded heterogeneities, etc.) Available multiphase flow codes use a number of constitutive models for retention and relative permeability functions. Systematic investigation of the adequacy and limitations of these constitutive models to the specific problem of DNAPL infiltration and distribution have not been reported in literature.

The primary goal of this work is to address the issue of which constitutive model or models better capture DNAPL infiltration and redistribution behavior in heterogeneous aquifers. Experimental data generated in intermediate scale test tanks was used in this evaluation.

2. EXPERIMENTAL APPROACH

All experiments were conducted in a tank with internal dimensions of 0.71m x 0.53m x 0.04m, with different combinations of homogeneous and heterogeneous soil packing configurations. The tank was packed to produce two distinct zones with an inclined interface (Figure 1). The goal was to create conditions where capillary barriers in combination with gravitational forces resulting in the DNAPL migrating laterally along the interfaces.

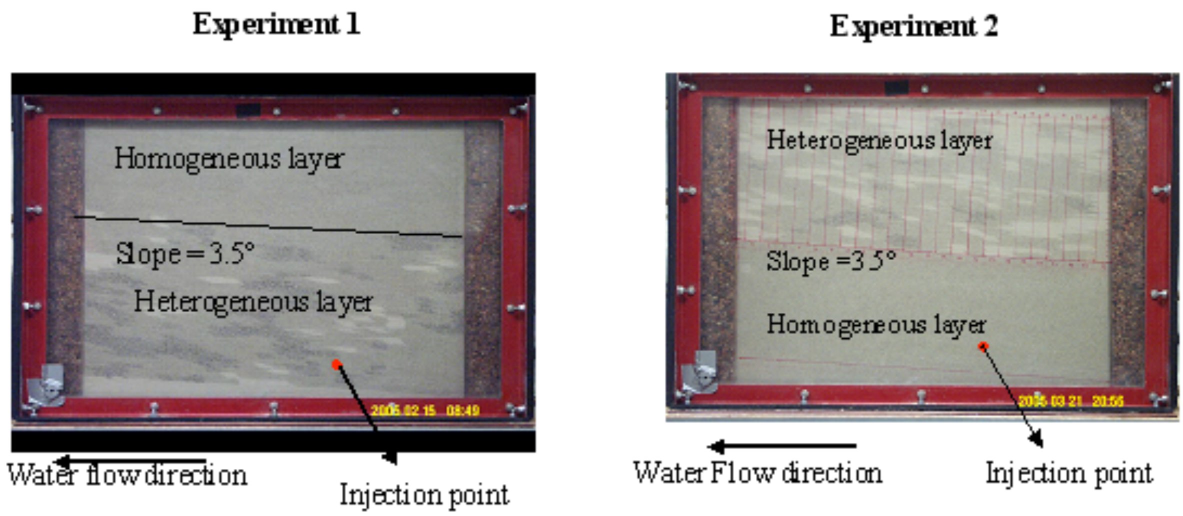


FIGURE 1. Heterogeneous fields used in the experiments

To avoid the generation of sands contaminated with toxic DNAPLs, a LNAPL was injected at the bottom of the tank to mimic the behavior of a DNAPL. Soltrol colored with Sudan IV hydrophobic organic red dye was used as the test LNAPL. In the first experiment, the upper zone was kept homogeneous and the second zone was packed to represent a spatially correlated random field with known geo-statistical parameters. In the second experiment, the two zones were reversed, making the upper zone heterogeneous and the bottom layer homogeneous. The interfaces within the two zones were designed with a dip of 3.5^0. The geo-statistical parameters used in the heterogeneous fields were: Lnk of -22.5 and -23.45 (k in m^2) for the first and the second experiment, respectively. A variance of 1 was used in both experiments. A head difference of 1 cm between the two end reservoirs was used to create steady groundwater flow across the tank. The fluid properties of Soltrol are: density = 810 kg/m^3, viscosity = 0.0048 Pa s and the interfacial tension between the water and Soltrol is 0.026 N/m. In the first experiment, 0.6 L of Soltrol was injected for 0.108 days at a constant rate. Similarly, in the second experiment 0.543 L of Soltrol was injected for 0.191days. The infiltration and redistribution of the Soltrol was monitored at different intervals through digital imaging and measuring the saturation distribution using an automated x-ray attenuation system.

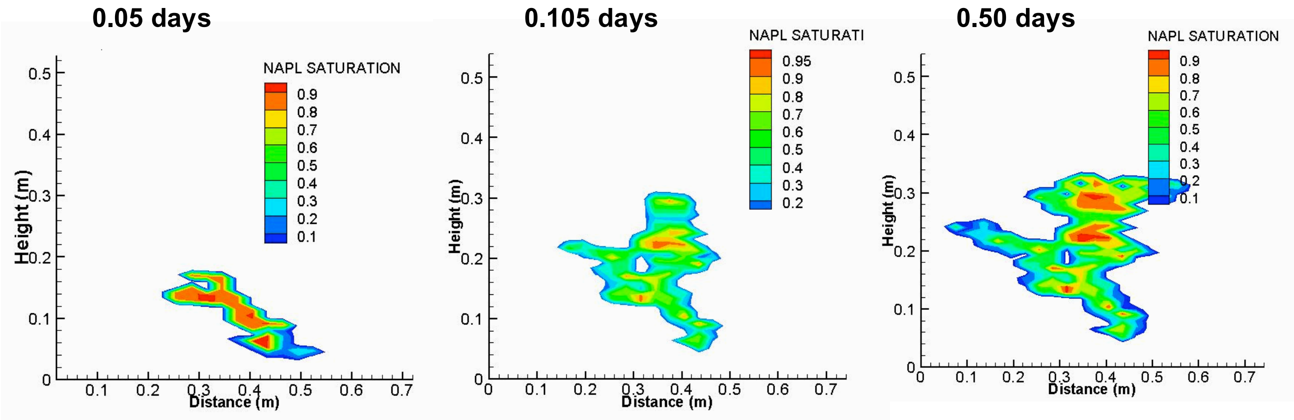
TABLE 1: Properties of the test sands used in experiments

Sand type	Permeability (k) (m^2)	Displacement Pressure -P_d (Pa)	Residual water saturation -S_{rw}	Porosity
# 8	1.93e-09	362.9	0.058	0.397
# 16	7.14e-10	474.8	0.058	0.389
# 30	2.25e-10	1030.0	0.057	0.394
# 50	4.32e-11	1667.7	0.110	0.355
# 70	2.69e-11	2589.9	0.150	0.396
# 110	7.30e-12	6376.5	0.280	0.323

3. SIMULATIONS AND DISCUSSION OF RESULTS

Most modeling studies reported in literature do not provide any insights to which constitutive models need to be used in available multiphase codes to accurately simulate different phases of DNAPL migration, such as infiltration and redistribution under heterogeneous conditions. In order to address this issue, detailed simulations were conducted for five representations of retention and imbibition behavior based on two commonly used constitutive models by Brooks and Corey (1964) and Lenhard and Parker (1987). The cases considered were: (1) Brooks-Corey (BC) drainage curve during injection and redistribution, (2) BC drainage curve during injection and BC imbibition curve during redistribution (3) Lenhard and Parker (LP) model with hysteresis, (4) LP model without hysteresis, and (5) BC drainage model with trapping during injection and redistribution (see Delshad et al., 1996 for detail).

All simulations were conducted using multiphase, multi-component flow and transport code UTCHEM9. This code was modified to incorporate hysteresis into the constitutive models and represent inclined layers of the packing. The model simulations of the five cases of constitutive model representations were compared against two experimentally observed behavior of NAPL infiltration and redistribution. Figure 2 provides a qualitative comparison of the model simulated NAPL saturation distribution using the first case of constitutive models (Figure 2a) and the experimentally observed distribution (Figure 2b). Figure 3 compares the simulated results at the end of 0.107 days for three cases where; (1) hysteresis was considered (case 3), (2) hysteresis not considered (case 4) and (case 3) effects of trapping considered (case 5). The cases 1 and 2 produced almost the same saturation distribution. The model simulated saturation distribution shows that during injection, case 1 model was able to match the experimental observations reasonably well. The simulated saturation distributions with and without hysteresis, and with trapping also qualitatively matched the experimental observations. The simulated and observed saturation distributions shown in Figure 2 also allow us to evaluate how saturation distributions change with time. The data shows that the model simulations matched better with the experimental observations when the time is lagged (e.g. 0.0785 simulation matches with the distribution observed at 0.079days). Although, there was this small time lag between the experimental and model results, all the constitutive models were able to simulate the migration pathways with reasonable accuracy. The observed profiles that were used in these comparisons were based on digital images. Further analysis is needed using more quantitative observations (x-ray data) to make final conclusion on the selection of best constitutive model to be used in simulating DNAPL infiltration.



(a) Model simulative distributions

(b) Experimentally observed distributions

FIGURE 2. Model and experimental results at different stages of experiment during infiltration and redistribution:

Figure 4a and 4b compare the model simulated and experimentally observed NAPL distributions 1 day after injection for three cases of the constitutive model representation (cases 1, 3 and 5). The simulated NAPL distribution for case 2 and case 4 almost matched with the NAPL distribution for case 1. None of the five cases considered was able to simulate the redistribution phase of DNAPL migration accurately. The model that allowed for hysteresis was able to approximately simulate the DNAPL pathway, but the distributions only matched with a 0.2 day time lag. The observed NAPL distribution at 1 day matched with the simulated saturation distribution of 0.8 days. During infiltration and redistribution, simulated distributions showed faster migration in comparison to the observations.

The model simulation was also carried out to compare with the observations of the second experiment. The same five representations of constitutive models were used. The model simulated NAPL distribution at 0.37 days using the constitutive models case 3 (LP with hysteresis) was compared to the observed profile observed at 0.4days. Similarly simulated distribution at 1.18 days was compared to observations at 1.4 days. As was observed in the comparisons associated with the first experiment, simulated saturation distributions for the second experiment also showed a time lag between the observations and simulations, especially during redistribution. The modeling results showed the same trends in simulating both experiments.

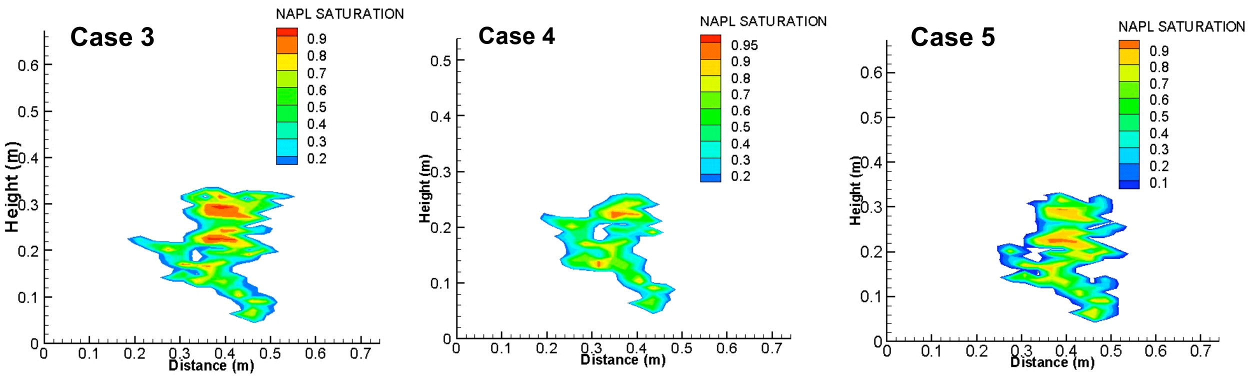


FIGURE 3. Effect of trapping and hysteresis on the DNAPL infiltration

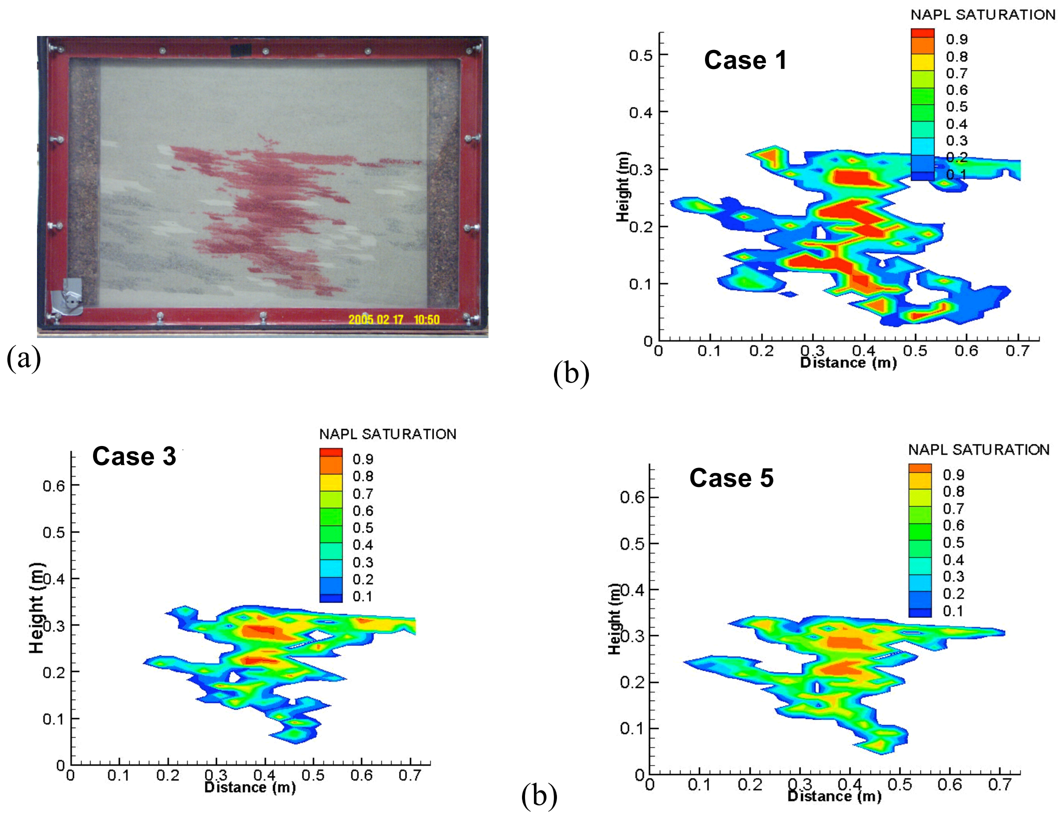


FIGURE 4. Observed (a) and simulated (b) NAPL redistribution at 1 day

4. CONCLUSIONS

The adequacy of available constitutive models for the simulation of DNAPL infiltration and redistribution were studied using results from controlled laboratory experiments conducted in intermediate scale test tanks. The simulations were conducted using different configurations of available constitutive models during infiltration and redistribution. Although there was a small time lag between the experimental and simulated results, all constitutive models selected for study were able to simulate the observed infiltration behavior reasonably well. All constitutive models simulated similar redistribution behavior, but the simulations did not match the experimental observations accurately. The model simulated saturation profiles matched the observations only with a time lag. The results also showed that the model simulated much faster redistribution compared to the observations. None of the selected representations of the constitutive models was able to match the observed redistribution behavior of the NAPL in the heterogeneous formations that were tested. This may be due to inappropriate constitutive relations, dynamic effect of capillary pressure (Hassanizadeh et. al, 2002; Manthey et. al, 2005) or micro- heterogeneity effects that were not incorporated into the simulations. Preliminary analysis shows that models that incorporate hysteresis gave better results than the models without hysteresis and with trapping, especially during redistribution. Further studies with quantitative data collected using the x-ray method will be conducted to make the final conclusions.

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