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An up-scaled, buoyant invasion percolation model for use in delineating subsurface DNAPL location

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Abstract

We introduce an up-scaled, buoyant invasion percolation model (UIP) for application to non-wetting, dense, non-aqueous phase liquid (DNAPL) migration at the geologic formation scale within the saturated zone of an aquifer. The UIP model incorporates a gravitational potential to model the displacement of fluids of different densities and can be used for either LNAPLs (lighter than water) or DNAPLs (denser than water). We demonstrate model behavior in a simulated braided stream deposit. Simulations show the influence of textural changes across layers and gravity forces in controlling DNAPL migration. While our results are encouraging, the application of this up-scaled percolation model requires a series of tests both in the laboratory and in the field before judgment of sufficient validity for its intended purpose is achieved.

Development of improved technologies for remediation of dense, non-aqueous phase liquid (DNAPL) spills cannot occur unless we also improve our ability to discover where DNAPLs reside in the subsurface. We propose a strategy incorporating probabilistic simulation of DNAPL location in the subsurface as a basis for optimal sampling. In this approach, multiple realizations of possible plumes from spill areas are combined to form a probability map of DNAPL location. Process-based simulations are performed in multiple realizations reflecting known information on subsurface conditions and spill history. Our uncertainty about the distribution of geologic features and the disposal history at the site can be propagated through the modeling to reflect the degree of uncertainty in DNAPL location. Having produced a probability map, an optimization algorithm that incorporates the probability map is used to guide the placement of additional characterization boreholes with the ultimate goal of reducing the uncertainty in DNAPL location to a level acceptable for a given remediation scheme. This approach is iterative; additional data are collected, geological simulations conditioned, flow model simulations conducted and probability map updated to be consistent with the new data.

A critical component of this approach is the modeling of DNAPL movement to its final locations within a given geologic realization. In this paper we consider the use of a percolation type model for macroscale DNAPL migration. Percolation models are considerably faster than standard two phase flow codes and therefore allow incorporation of more geologic detail. We expect that detail with respect to textural changes within and across geologic units will be vital in the prediction of non-wetting, dense fluid migration. We begin by describing the current pore scale form of percolation models. We then present an up-scaled buoyant invasion percolation model for application to meso-scale sedimentary units. Model behavior is demonstrated in a two-dimensional cross section of a simulated braided stream deposit.

PORE AND UP-SCALED PERCOLATION MODELS

Under most natural-gradient conditions, DNAPL movement through the saturated zone will be controlled by gravitational and capillary forces. This presumes that flows are sufficiently slow that viscous forces are small with respect to gravity and capillarity. For such conditions, laboratory studies suggest that for non-wetting DNAPLs, pore scale behavior leads to capillary fingering in horizontal "homogeneous" micromodels [1] and an interplay of gravity fingering and capillary fingering in non-horizontal systems [2]. For both of these situations, forms of percolation theory can be used to model the immiscible displacement process at the pore scale.

Standard percolation (SP), introduced by Broadbent and Hammersly [3], assumes full thermodynamic equilibrium between phases and across a network of connected pores. Assuming that each individual pore is equally accessible to both phases (capillary bundle theory), phase occupancy, or which pore is filled with which fluid, is determined solely by the pore distribution. While this theory has proven to be quite useful for modeling phase changes and critical phenomena, due to requirements of connection within phases for flow, it is of limited use for modeling incompressible, two-phase, immiscible fluid displacements in porous networks (e.g., porous media). To more adequately represent fluid-fluid displacements in porous networks, Wilkenson and Willemsen [4] intro

duced *invasion percolation* (IP) which incorporates phase accessibility rules to assure that connectivity within phases is considered in the pore filling criteria. Here, connection to the source of the invading phase is a condition for invasion. In addition, the defending fluid must be able to exit the pore to its sink or the pore may not be invaded and is thus entrapped within the invading fluid.

IP must be implemented numerically. First, a pore network of given connectivity is generated such that each pore is assigned a radius selected from a given distribution. Certain pores are then filled with the invading fluid at the boundary surface, often either an edge of a rectangular network or a disk at the center. All pores connected to the invaded pore surface are available for filling and the one with the highest assigned probability of invasion (based on the pore radius) is found and filled. This action adds new pores to those available for invasion and the modified list is next sorted to find once again the pore with the highest assigned probability of invasion and so on. Pores that become entrapped may or may not be removed from the pores available to be filled depending on the situation of interest. If the defender fluid is incompressible or nearly so, then removal is appropriate. Conversely, if the defender fluid is infinitely compressible or will dissolve in the invading phase then entrapped pores should not be removed. An example of IP on a two-dimensional pore network with connectivity of four (i.e., each node is connected to four others, right, left, up, down, on a checkerboard grid) and phase trapping is shown in Figure 1a.

IP has been applied to immiscible flow in porous media by a number of researchers [5] and has been shown to effectively model displacements in two-dimensional pore networks in micromodels where a non-wetting fluid invades a wetting fluid [4]. For wetting fluid invasion, macroscopic fronts typically form and IP must be modified to reflect interfacial smoothing induced by pore geometry [6, 7, 8]. An example of wetting invasion on the identical network as in Figure 1a is shown as Figure 1b. In non-horizontal networks, gravitational potential must also be included. Addition of gravitational potential allows both the simulation of capillary rise and gravity-driven fingering with both the rise height and finger width adequately simulated by the modified invasion percolation (MIP) model [6, 7, 8]. Figures 1c and 1d show the influence of gravity included in the MIP model for both non-wetting and wetting fluid invasion.

Pore scale behavior yields two important macroscopic effects. The first is a well defined percolation threshold pressure and the second is a phase entrapment saturation when either phase becomes discontinuous within the other. These macroscopic effects are critical for defining an up-scaling of invasion percolation. When the percolation pressure is reached, the invading phase spans the system and fills the majority of pores. After this point, as the pressure is increased the phase continues to enter the system until the defending phase is cut off from the system outlet and becomes fully entrapped.

Up-scaled Invasion Percolation Model

In order to apply MIP at the macroscopic scale, we conceptualize the physical system as an ensemble of homogeneous isotropic porous media blocks, each of which has well defined pressure/phase saturation curves. The pressure/saturation relation has two distinct points of importance, the wetting phase satiation pressure and the non-wetting phase entry pressure. The fact that these two pressures are different demonstrates the significant hysteresis intrinsic to two-phase flow in porous media.

The non-wetting fluid entry pressure relates to the largest pore along the phase entry interface. This entry pressure must be attained by the invading fluid prior to invasion of the individual block. To span the block, the pressure must be increased to the percolation threshold pressure discussed above. At this pressure the block is spanned but not filled. Once the block is spanned, the invading phase comes in contact with the surrounding blocks and will readily enter them if their entry pressures are lower than that achieved to span the first block. However, if the pressure is not high enough to enter any of the adjoining blocks, the block continues to fill (increase non-wetting phase saturation) until it reaches the entry pressure for one of the adjoining blocks. The maximum non-wetting phase saturation that can be achieved in any block is the satiated or fully entrapped wetting phase saturation value where the wetting phase can no longer exit the block.

The drainage of non-wetting phase from individual blocks proceeds as the pressure within the system drops below the wetting fluid entry pressure where water can first enter the block. Once the pressure has dropped below the percolation threshold pressure for the wetting fluid, the block is spanned and adjacent blocks can now be entered. As pressures in the network decrease, non-wetting fluid saturations drop to the residual value where the non-wetting phase is entirely trapped by the wetting fluid.

At the block scale, the critical pressures to model are the phase percolation pressures as they determine block invasion and thus the phase connection within the network of blocks. Cast in terms of a potential, the capillary pressure potential, Ψ_c, is given by

$$\Psi_c = -\frac{2\sigma\cos(\alpha)}{\rho_o g R} \qquad (1)$$

At the block network scale, gravity forces will be immediately important as the invasion progresses. To incorporate gravity forces, we calculate a total phase entry potential, Ψ_t, as the sum of the critical capillary pressure potential and gravity potential given as hydrostatic:

$$\Psi_t = \Psi_c + \Psi_g \qquad (2)$$

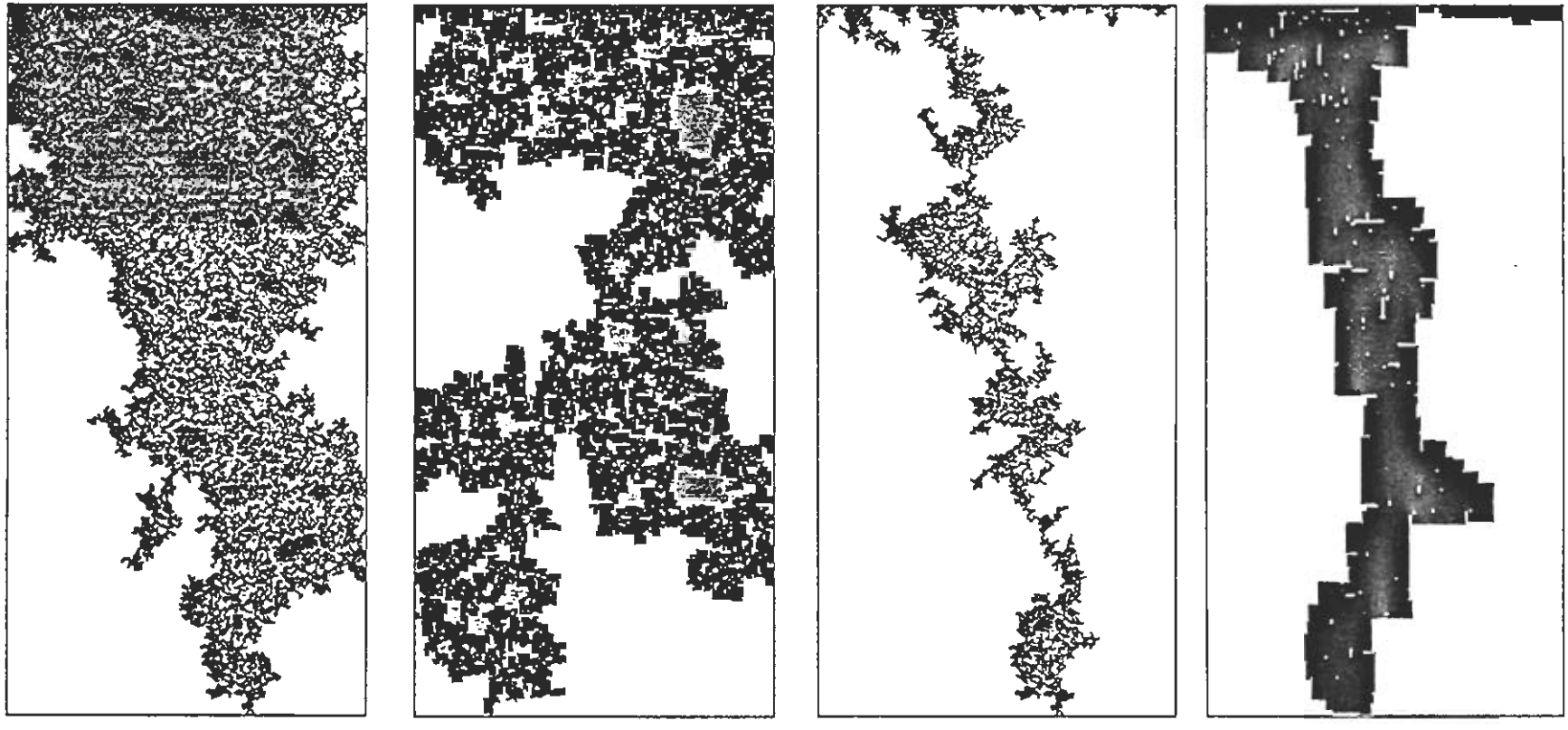

Figure 1: General behavior of invasion percolation type models applied at the pore scale. For all models, the identical pore network was used with a connectivity of 4 and phase trapping included. a) IP (horizontal, non-wetting fluid invasion) b) MIP (horizontal, wetting fluid invasion), c) IP with gravity (vertical, non-wetting fluid invasion), d) MIP (vertical, wetting fluid invasion). The invading fluid enters the network from the top and the figures show the phase occupancy at network breakthrough (percolation threshold pressure). The invading phase is denoted with black, the defending unentrapped phase with white and the entrapped defending phase with gray.

Since the gravity potential is simply equal to the downward distance into the network from the spill point we have

$$\Psi_t = -\frac{2\sigma\cos(\alpha)}{\rho_o g R} - z \qquad (3)$$

Implementation of this up-scaled invasion percolation model (UIP) requires the definition of a network of R including its connectivity and individual R values for each block across the formation scale field. Resolution in z is critical. Increments in z must be lower than local perturbations in Ψ_c due to property variation so that artificial gravitational effects do not overwhelm model behavior. An invasion percolation algorithm identical to that at the pore scale discussed above, is then implemented. A critical component of UIP application is the proper representation of the geologic media as will be discussed in our demonstration below.

DEMONSTRATION OF UP-SCALED PERCOLATION MODEL

We demonstrate the behavior of UIP in the context of a realistic geologic simulation of a braided-stream deposit similar to those expected along many rivers where industrial activity is concentrated. We implement UIP simplistically in a two-dimensional cross section with a network of connectivity four. We assume that once the percolation potential is achieved in a block, it fills to the satiated value. Furthermore, trapping at the block scale and drainage of the non-wetting phase is not considered in this demonstration.

Geologic Simulation

The arrangement of petro-physical properties used as a basis for this UIP demonstration was derived from a mixed geometric and process-based geological simulation model known as the Braided Channel Simulator (BCS-3D) [9]. BCS-3D is designed to simulate the three-dimensional spatial distribution of sedimentary facies developed by a laterally confined braided-stream system [10]. Post glacial sediments of this type are common in valleys of the northern mid-west and north-eastern United States, Canada, and much of Europe.

The BCS-3D simulation presented here used the facies description of Brierley [11] for the Squamish River, British Columbia and was calibrated to the braided topography of the Ohau River, New Zealand described by Mosley [12] (see [9] for details). The BCS-3D simulation consists of 10 discrete units in a 150 by 150 node square, 100 nodes deep. Nodes denote volumes of 3 m by 3 m square by 0.05 m deep (a vertical exaggeration of 60 to 1). The output was subsequently processed to impose a non-overlapping random uniform distribution within each unit. Finally, for the current demonstration purposes, a two-dimensional slice perpendicular to the direction of fluid flow (transverse to channels) was extracted for use in the UIP simulations (see figure 2). To limit the effect of boundary conditions where the braided pattern is poorly represented by BCS-3D, 10 columns of nodes were removed from both ends of the cross section.

Percolation Model Simulations

Units from geological simulation are mapped into the reference critical pore radii (R) field as shown in Table 1. This mapping covers the range of expected R values for braided stream deposits. To explore two additional capillary scale similar formations each representing on the whole finer or coarser textures, the reference R field is multiplied by a "formation" scale factor of .25 or 4.0, respectively. For demonstration, we consider PCE as the DNAPL so that σ is 41.8 dynes/cm, ρ_o is 0.61 g/cc, and α is 180 degrees. At the top of the water saturated formation, DNAPL is released at 4 spill locations. From each of these locations, UIP begins and continues until the bottom of the network is encountered. Water is allowed to exit the network across any of its edges.

A connection of 4 was used for the UIP simulations. Figures 3a, 3b, and 3c depict the results from UIP simulations for formation scale factors of 4.0, 1.0 (reference field), and 0.25, respectively. Each of the four spill locations are superimposed in the figures. Once a path from one spill location simulation intersects that from a separate spill simulation, the DNAPL follows an identical path to the bottom of the formation.

DISCUSSION

Simulations indicate that once a unit is entered, DNAPL essentially falls in a one node wide "finger". Once the finger finds the bottom of the unit, the finger either continues down though the next unit (next unit has larger pores) or fills the unit up (next unit has smaller pores) depending on the phase percolation potential. Unit filling occurs until either sufficient potential to enter the adjacent lower unit is achieved or another unit is encountered to the side where the DNAPL has sufficient potential to enter and it then "spills over" the impeding unit and goes around. Both of these effects are in qualitative agreement with heterogeneous micromodel experiments conducted by Wilson et al. [2].

The interplay of gravity and formation capillary scale factor greatly affects where the DNAPL goes. As the formation capillary scale factor is decreased (differences between unit phase entry potentials decrease), gravity dominates and DNAPL moves through the formation as a single finger (figure 3a). As the formation capillary scale factor is increased (differences between unit phase entry potentials increase), DNAPL movement is influenced much more by textural interfaces and forms a series of pools connected by fingers (figure 3c). In addition, DNAPL movement seems to be focused by the formation with three of the four spill locations joining in Figure 3b and 3c for the smaller formation scale factors. Whether

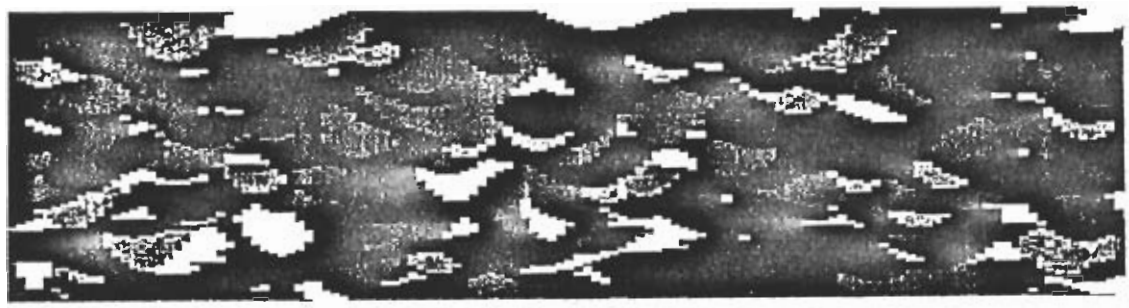

Figure 2: Geologic cross-section of braided stream deposit used in demonstration UIP simulations at a vertical exaggeration of 20 to 1. Gray scale denotes units 1 (black, finest) to 10 (white, coarsest). Note that units 1 and 2 are not found in this cross-section and that R increases with unit number (see Table 1).

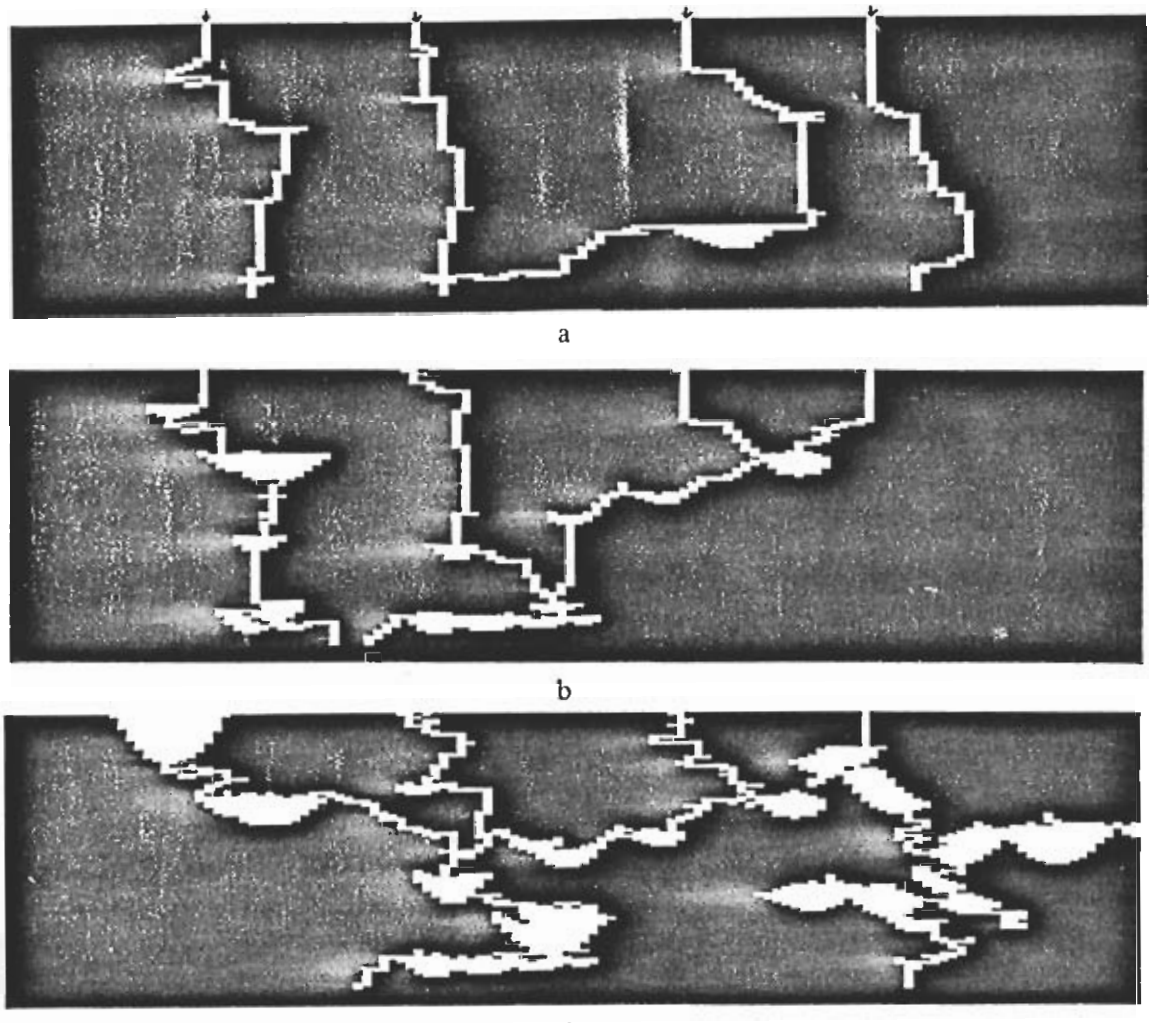

Figure 3: UIP simulation with capillary formation factors of a) 4.0 (coarsest), b) 1.0 (reference), and c) 0.25 (finest), using the geology depicted in Figure 2. The results of simulations from 4 points along the top of the formation (arrows) are superimposed with black denoting water and white DNAPL invaded blocks.

TABLE 1

unit #	% of each unit in section	reference unit R (cm)	UNIT PHASE CRITICAL POTENTIAL (cm) scale factor 4	scale factor 1	scale factor.25
10	1	1.00E-01	3.48E-01	1.39E+00	5.56E+00
9	2	4.50E-02	7.73E-01	3.09E+00	1.24E+01
8	10	2.00E-02	1.74E+00	6.95E+00	2.78E+01
7	22	8.75E-03	3.97E+00	1.59E+01	6.35E+01
6	40	3.75E-03	9.26E+00	3.70E+01	1.48E+02
5	14	1.56E-03	2.22E+01	8.89E+01	3.56E+02
4	6	6.25E-04	5.56E+01	2.22E+02	8.89E+02
3	4	2.34E-04	1.48E+02	5.93E+02	2.37E+03
2	0	7.81E-05	4.44E+02	1.78E+03	7.11E+03
1	0	1.95E-05	1.78E+03	7.11E+03	2.84E+04

this focusing is an artifact of the geological simulator, the use of only a two-dimensional slice from the geological simulation, or due to something intrinsic in braided stream deposits must be further investigated.

In our demonstration simulations, we chose facies R values (Table 1) that were reasonable based on limited pressure/saturation data from geologic deposits. We varied the formation scale factor in an effort to understand how differences in R values across units influence DNAPL movement in relation to gravitational forces. Much additional work including both measurements of saturation/pressure relations and pore scale IP or MIP modeling is required to properly predict R for a variety of geologic deposits.

A number of enhancements to the UIP code as well as a series of tests to determine whether UIP adequately models DNAPL movement within the saturated zone are in progress. The model has been extended to three dimensional networks and we are beginning to consider the drainage process so that correlation between spill volume and migration can be made. In addition, the sensitivity of simulations to the geologic simulator and choice of facies R values (overlapping or not) is being considered.

Critical to the valid application of UIP to spill migration problems is the comparison of model predictions and nature. To accomplish this, we are conducting controlled laboratory experiments in heterogeneous sand slabs where DNAPL is spilled on the top surface. An example of a heterogeneous sand slab is shown in Figure 4. Experiments make use of light passage techniques that allow two-dimensional DNAPL saturation fields to be measured using digital imaging technology [13]. Heterogeneity will be systematically varied to challenge the UIP model. In the process of testing UIP model validity, we will also consider the ability of standard two-phase flow codes to capture physical system behavior.

CONCLUSION

We introduce an up-scaled version of invasion percolation for application at the formation scale for non-wetting DNAPL invasion. The UIP model incorporates a gravitational potential to model the displacement of fluids of different densities and can be used for either LNAPLs or DNAPLs. Demonstrations of the model on a simulated braided stream deposit show the influence of textural changes across layers and gravity forces in controlling DNAPL migration. While these preliminary results are encouraging, further application of this up-scaled percolation model requires a series of tests both in the laboratory and in the field to judge its validity for the intended purpose.

ACKNOWLEDGMENTS

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NOTATION

- σ surface tension between phases
- ρ_o the differential fluid density (ρ_1-ρ_2)
- α contact angle between advancing and defending phases (0 for fully wetting, 180 for fully non-wetting)
- g gravitational acceleration
- R critical pore radius for phase percolation

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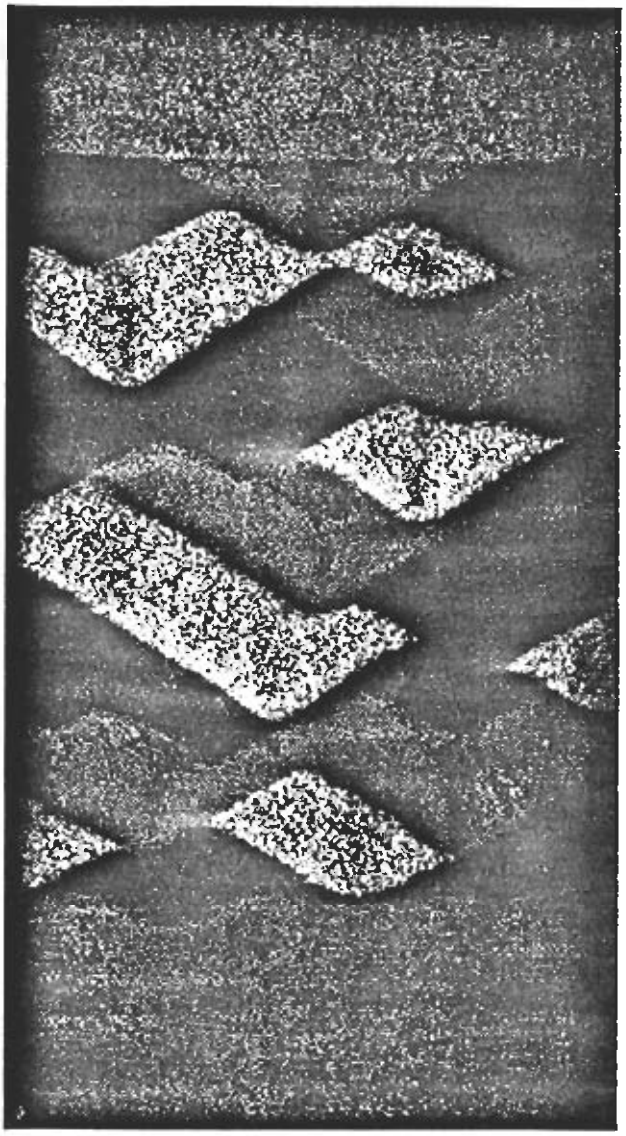

Figure 4: Heterogeneous sand slab (1 cm thick, 30 cm wide, 60 cm tall) as visualized using the digital image based light transmission technique. Three units are embedded in a structure similar to Figure 2. Lightest are coarsest, largest R units, darkest are finest, smallest R units. Experiments in structures such as this will be used to test the validity of the UIP model.

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