Flow Visualization and Processes Laboratory

DNAPLs <u>(dense non-aqueous phase liquids)</u>

Problem

Spilled chlorinated organic solvents have created pervasive groundwater contamination problems because of their ubiquitous use, their toxicity and persistence within the environment, combined with the difficulty in recovering them from the subsurface. These solvents are immiscible with water and more dense than water. It is for these attributes that they are commonly referred to as DNAPLs (dense non-aqueous phase liquids). They migrate downward through aquifers as a separate phase, travelling under the combined influences of gravity and capillary forces.

Background

Variations in media texture that the DNAPLs encounter as they migrate can have a profound influence on the migration path. It is the interplay between gravity, capillarity and these textural heterogeneities that complicates the migration of the DNAPLs and therefore it is not straightforward to predict the locations in the aquifer at which the spilled DNAPLs may ultimately reside. Uncertainties in the region of solvent contamination translate into higher remediation costs as the remedial system must be designed in light of these uncertainties.

Variations in texture can have profound effects on migration. At the majority of spill sites, we may never have sufficient geologic detail. Significant uncertainties in the exact configuration of facies assemblages tend to limit the utility of deterministic modeling approaches. Therefore, we have developed a probabilistic modeling approach that uses Monte Carlo simulation of DNAPL migration through 3-D geologic fields

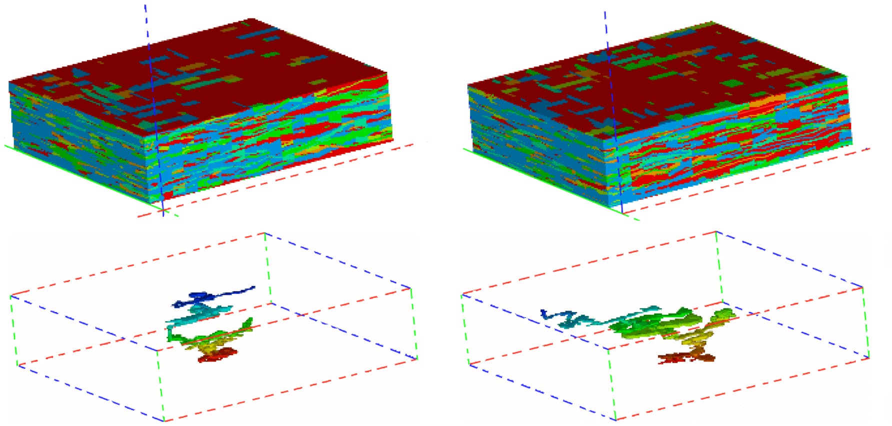

Figure 1. Geologic simulations (top) are combined with upscaled invasion percolation models (bottom) of DNAPL migration to produce probability maps of potential DNAPL locations.

to produce a probability map of potential DNAPL location. In this approach, multiple simulations of DNAPL migration capture the physics of DNAPL movement through the geologic features controlling DNAPL migration (figure 1). Our simulations yield realistic results with the DNAPL configured into fingers and pools corresponding to the effects imposed by the textural variations between geologic facies. In creating the probability map, we quantify uncertainty about the distribution of geologic features and the disposal history at the site and propagate these uncertainties through the modeling to create a map that reflects the degree of uncertainty in DNAPL location. The probability map can then be used to guide characterization activities (Borchers et al., 1995).

In developing an integrated framework for tackling the DNAPL location problem, we identified the lack of fast DNAPL migration models as a barrier to implementation of our approach. (Continuum multiphase flow codes carry too large a computational burden to be used in Monte Carlo analyses.) To fill this gap, we developed and implemented an upscaled invasion percolation model to simulate macro-scale DNAPL migration (Glass et al., 1995). Previously, percolation models have been used exclusively to model pore-scale displacement processes. To apply a percolation approach to modeling DNAPL migration from a spill site, we proposed a procedure to upscale the model from the pore scale to the geologic scale of interest. This upscaling of percolation models represents a novel approach to modeling field-scale migration phenomena. Such models offer several advantages over multi-phase flow codes currently in use. First, unlike multi-phase flow codes, percolation codes are able to model gravity-driven fingering, an important unstable displacement process and a common feature of DNAPL migration. Second, because percolation models neglect viscous forces, the data requirements are much lighter and the computations are speedy enough for the code to be run using a Monte Carlo approach while incorporating geologic heterogeneities on a much finer scale. Because of inherent geologic complexity and uncertainty, deterministic modeling is rarely able to provide useful insight about the extent of DNAPL migration.

Migration Experiments

Preliminary model verification experiments conducted in the laboratory with a limited set of heterogeneity and fluid parameters have yielded extremely encouraging results (Conrad et al., 1995). As one example, figures 2 and 3 compare the downward infiltration of TCE through a water-saturated sand pack (figure 4) with the results of the invasion percolation model. The model closely follows the path and general shape of the lab experiment. Similarities in color distribution between model and experiment indicate that the model closely predicts the progression of TCE migration. The model slightly over-predicts the amount of TCE pooling above a fine sand barrier in the experiment (which appears as a dark line slightly lower

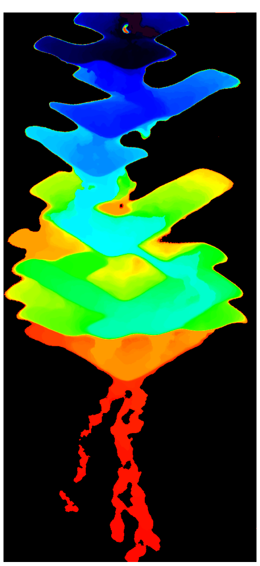

Figure 2. Downward infiltration of TCE through a hetrogeneous, water saturated sand pack.

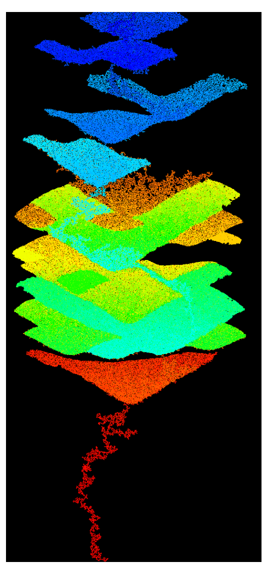

Figure 3. Downward infiltration of TCE through the sand pack as predicted by the percolation model.

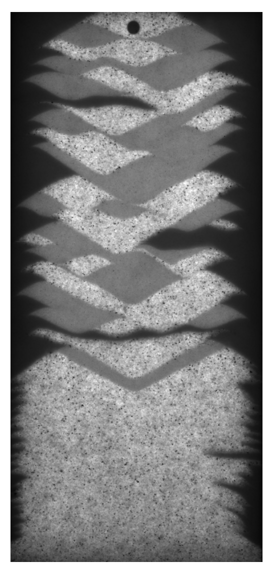

Figure 4. Thin sand slab (30x60x1 cm thick) is packed using a computer controlled apparatus to yield a reproducible and controlled heterogeneity structure.

than halfway down the image). However, excellent agreement of the modelling results to the experiments provides an initial indication that upscaled percolation models may adequately represent the physics of DNAPL migration.

Remediation Experiments

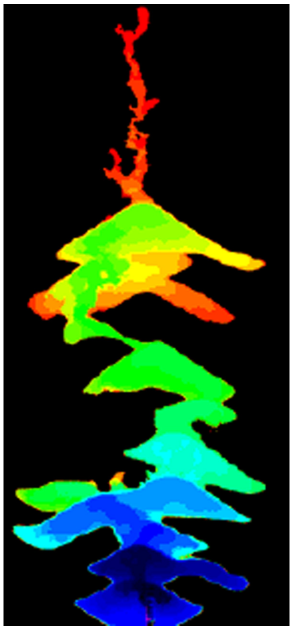

Figure 5. Soltrol 130, a DNAPL analogue, was used in this experiment to observe effects of changes in interfacial tension.

Recently, we have begun to extend our laboratory work to consider remedial processes. In an effort to clean up spilled DNAPLs, several remediation approaches are currently under development. Chemically enhanced solubilization, alcohol displacement, and air sparging are among the most promising. Many of these techniques have undergone preliminary field demonstrations. However, results from such field demonstrations cannot be extrapolated to predict remedial performance under the wide range of field conditions encountered at spill sites. In addition, these techniques have not yet been sufficiently tested and quantitatively compared in well -controlled laboratory experiments under heterogeneous conditions indicative of what can be expected in the field nor have the numerical simulation techniques used to predict DNAPL migration and remediation treatments been adequately verified through comparison against laboratory experiments conducted in heterogeneous media.

Because pilot scale experiments at existing spill sites are irreproducible and difficult to interpret, we are in the process of implementing well-controlled experiments in the laboratory to compare a series of remediation techniques on the same identical system. This requires that the heterogeneities we create in the lab be: 1) representative of nature; 2) able to be varied in a controlled fashion; and, 3) reproducible. We also need to be able to "see what is going on" within the full system as well as simply measuring gross system response (i.e. outflow concentrations). As examples, we will need to be able to observe the nature of flow instabilities as air bubbles up through the formation during air sparging, or during a surfactant flood, we will need to directly observe the point at which interfacial tensions have become low enough to induce significant downward mobilization of previously trapped DNAPL. The quantitative visualization techniques based on transmitted light developed at the FVPL (Tidwell and Glass, 1994) are ideal for observing such processes.

Publications

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