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Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

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Research Objective

The goal of our research is to develop a fundamental quantitative understanding of the role of physical heterogeneities on DNAPL migration and remediation in aquifers. Such understanding is critical to cost effectively identify the location of the subsurface zone of contamination and design remediation schemes focused on removing the source of the contamination, the DNAPL itself. To reach this goal, the following objectives for the proposed research are defined:

Objective 1: Develop fundamental understanding of the physics of DNAPL migration processes within heterogeneous porous media: a) Conduct a suite of two-dimensional thin slab physical experiments within controlled and systematically varied heterogeneous porous media at scales up to one meter. Vary system parameters to consider a range of capillary and bond numbers within these heterogeneous porous structures. b) Develop a new DNAPL migration model based on an Up-scaling of Invasion Percolation (UIP) to model the migration process. Compare the model predictions to experimental results. Accomplishing objective 1 provides a series of experiments against which we will be able to evaluate the validity of existing multi-phase flow theory as formulated in both percolation codes and in continuum flow codes. These experimental results will also provide new insights into DNAPL migration behavior. Development of the UIP model will provide an exciting alternative to continuum multi-phase flow codes since UIP offers several advantages for modeling DNAPL migration. The UIP model is fast, allowing for: 1) modeling in three dimensions; 2) the incorporation of much more geologic detail; and, 3) its use in probabilistic modeling by way of Monte Carlo techniques. In addition, the UIP code requires much less input data and it can handle density-driven fingering, a process known to occur with DNAPLs.

Objective 2: Develop fundamental understanding of the physics of DNAPL remediation processes within heterogeneous porous media: Conduct a suite of physical experiments within controlled and systematically varied heterogeneous porous media at scales up to one meter that consider surfactant and alcohol flushing and possibly air sparging remediation treatments. Accomplishing objective 2 will allow us to consider the efficacy of several promising DNAPL remediation techniques under realistic yet well-controlled conditions. We consider this work to be of the type of broad-based, initial studies needed to better understand the intricacies associated with various remedial processes. We expect that the results of this work will be used to focus subsequent research on those remedial approaches or combination of approaches that appear to offer the most promise.

Research Progress and Implications

This report summarizes work after 21 months of a 36-month project.

Objective 1: Develop fundamental understanding of the physics of DNAPL migration processes within heterogeneous porous media.

Our approach integrates experimentation using unique capabilities at SNL's Flow Visualization and Process Lab with development of new approaches for modeling DNAPL migration. Our experimental system consists of a 2D, sand-filled, initially water-saturated chamber (60cm high, 30cm wide, 1cm thick) where we can fully visualize DNAPL migration using light transmission techniques. Image analysis tracks the differences in light intensity for each successive image thereby yielding a time series of the displacement process at exceptional spatial and temporal resolution. Such resolution allows us to perform detailed data analysis that is sufficient to increase our understanding of DNAPL migration processes and to test our upscaled percolation model. In order to make reproducible geologic structures for our experiments we use a unique computer-controlled sand-filling apparatus. With our filler we can make macro heterogeneities (such as discrete formation-scale features like facies) as well as smaller scale micro heterogeneities (such as micro layering and crossbedding found within lithologic units).

Our percolation model neglects viscous forces. DNAPL migration is entirely dictated by local capillary and gravity forces as applied at scales on the order of centimeters. Percolation models simply track growth order (instead of solving for a pressure field at each time step) resulting in very fast computations. The speed of the model allows much more detail about heterogeneities to be incorporated. The UIP model easily models gravity driven fingering, a process common to DNAPL migration. Data requirements for the UIP model are light and readily obtainable. All that is needed is DNAPL density and interfacial tension, and the boundaries of lithologic units and their textures.

In macro-heterogeneous fields, we have conducted a suite of immiscible displacements through heterogeneous porous media in which we vary system parameters to consider DNAPL migration over a range of capillary and Bond numbers. All our experiments clearly show the invasion field to evolve in a series of gravity stabilized and destabilized invasion periods resulting in a final configuration of fingers and pools. We also have discovered pulsation within the flow field and the formation of multiple fingers even at low capillary numbers. These phenomena are important as they can result in more complicated migration behavior. With the exception of these effects, our UIP modeling shows good agreement to experiment even for increases in capillary number of over 2 orders of magnitude. The implication of these encouraging results is that the negligible viscous effect assumption in the percolation model will probably not be violated for the vast majority of DNAPL spill situations.

We have also begun to explore the effects of micro heterogeneities (such as micro layering and crossbedding found within lithologic units). In an initial series of experiments, microstructures have been varied through their “intensity” in terms of property variation across individual laminae. Results obtained suggest that the degree of small-scale heterogeneities affect effective block saturations and may well affect accessibility rules for the upscaled percolations. Additionally, in these laminated systems we see that effective block saturations are much more sensitive to flow rate than in either homogeneous systems or in discrete/macro-scale systems that we have studied. Percolation modeling of these experiments is in progress.

Additionally, a set of UIP enhancements are under consideration for: 1) the simultaneous invasion of both wetting (water) and non-wetting (DNAPL) phases (rudimentary model currently implemented); 2) incorporation of viscous forces (multiple fingers and greater “fill in” of migration field); and 3) dynamic time-varying contact angles.

Objective 2: Develop fundamental understanding of the physics of DNAPL remediation processes within heterogeneous porous media.

Simulators of remediation processes have not been extensively tested, in part due to the general lack of results from controlled experiments. Verified simulators of remediation processes are sorely needed as remedial selection and design tools. And since sufficient geologic detail is almost always lacking, it is important to understand the errors introduced through paucity of geologic detail.

Through our work on DNAPL migration, we have developed a unique experimental system where we can reproduce complicated heterogeneity structures. This system also allows us to conduct experiments for the first time that can compare several competing approaches for DNAPL remediation on equal footing. The combination of DNAPL migration studies and DNAPL remediation studies is also critical in that we can provide realistic initial DNAPL emplacement conditions for the remediation experiments. We emplace the DNAPL through a migration experiment as performed within the context of objective 1, followed by a remediation experiment.

We have completed construction of a 60cm x 60cm chamber required to run the remediation experiments. Design and construction of this chamber was complicated by the weight of the chamber and the additional ports required to run the remediation experiments. We have established a protocol - explicit, detailed procedures - for conducting these remediation experiments. We have purchased a gas chromatograph to measure effluent concentrations from the experiments and expect to run our first remediation experiment - surfactant solubilization - in the July/August 1998 time frame.

We intend to work closely with developers of each remediation approach to attempt to optimize the remedial process and show each technique in its best possible light. These experiments will be extremely useful to the remediation developers in helping them understand the physics and chemistry of their remediation processes as they perform under more realistic, less idealized, conditions. Toward that end, Alex Meyer, a professor at Michigan Tech, visited our lab and is collaborating with us on our first series of experiments looking at surfactant mobilization and solubilization of DNAPLs.

Planned Activities

We are in the process of completing data analysis and percolation modeling of all our DNAPL migration experiments. Through the end of this calendar year, we will be writing papers describing our research results.

This Summer we begin running our remediation experiments. We expect to continue running remediation experiments through the Spring of 1999 and write a series of papers describing results through the end of our funding in September 1999.

We anticipate funding beginning in FY 1999 from EM-50's Subsurface Contamination Focus Area for the purpose of conducting an extensive field application of our upscaled percolation modeling approach for locating DNAPLs. This funding will help provide the link from the basic science we have been performing in the EMSP to wide-spread application at DOE field sites.

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We have completed a paper that describes how our upscaled percolation model can be used within a Monte Carlo analysis to help determine DNAPL location by creating a probability map of where the DNAPLs might reside. Such a map could be used in conjunction with any DNAPL detection technology to suggest the most profitable sampling locations. Contact us to receive a copy. The citation is:

Borchers, B., S.H. Conrad, E.K. Webb, R.J. Glass Jr., R. Cox. 1997. A simulation and decision analysis approach to locating DNAPL in subsurface sediments. Sandia Report SAND97-2261.