YEAR ONE REPORT

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Title: Partitioning Tracers for In-situ Detection and Quantification of Dense Nonaqueous Phase Liquids in Groundwater Systems.

Project Number: DE-FG07-966ER14722

Program: U.S. Dept. of Energy Environmental Science and Management Program

Goal and Objectives:

The overall goal of the proposed project is to explore the use of partitioning tracers to characterize dense nonaqueous phase liquids (DNAPLs) in subsurface systems. Bulk-phase partitioning tracers will be investigated to detect and determine DNAPL saturation, while interface partitioning tracers will be investigated to measure the area of the DNAPL-water interface. The specific objectives that will be addressed to accomplish this goal are:

1. Investigate the use of partitioning tracers to detect and determine both the saturation and interfacial area of DNAPLs in saturated porous media.

2. Investigate the effect of rate-limited mass transfer on the transport behavior of partitioning tracers.
3. Investigate the effect of porous-media heterogeneity on the transport behavior of partitioning tracers.
4. Develop and evaluate mathematical models capable of simulating the transport of partitioning tracers in complex systems.

Summary:

One-meter Flow Cell

A meeting was held at the University of Arizona in August, 1997 between Mark Brusseau (principal investigator), Mart Oostrom (co-investigator from PNL), Nicole Nelson (graduate student), Tyson Carlson (undergraduate student) and Jim Szecody (PNL). The purpose of this meeting was to deliver a stainless-steel flow cell to the University of Arizona from PNL. During this 3 day meeting experiments were planned and use of the flow cell was demonstrated. The flow cell was packed with sand and a preliminary dye experiment was conducted to help develop sampling methods, a good packing technique and to chose experimental parameters such as flow rates and sampling frequency. This system wil1 be used to help examine the impact of porous-media heterogeneity on the performance of the partitioning tracer method. Results from the experiments will also be used to help design experiments to be conducted in the intermediate-scale flow cell discussed below.

Intermediate-scale Flow Cell

An intermediate-scale flow cell has been designed and constructed as a part of this project. This flow cell will be used to examine the impact of water and NAPL saturation distribution, as well as porous-media heterogeneity, on the performance of the partitioning tracer method. The flow cell, the dimensions of which are 1.8 m x 1 m x 0.05 m, is designed to be fully compatible with an existing dual-energy gamma radiation system. Water and residual NAPL saturations can be measured simultaneously with this system. One side of the flow cell is made of glass, to allow flow and transport visualization. The other wall is made of Kynar, a DNAPL-resistant plastic. The Kynar can be easily machined to install sampling ports at any desired lotion. A meeting was held at the University of Arizona in March of 1997 between Mark Brusseau (principal investigator), Mart Oostrom (co-investigator) and Nicole Nelson (graduate student) to design experiments to be conducted in the flow cell during the upcoming year.

Lysimeter

Both gas-phase and aqueous-phase partitioning tracer experiments will be conducted in a large (250 cm ID by 400 cm deep) weighing lysimeter. The lysimeter is densely instrumented with pressure transducers, TDR probes, tensiometers, and ports for aqueous, gas, and soil sampling. This design allows detailed monitoring of system parameters. The weighing capability allows a complete mass balance to be maintained through out an experiment. A preliminary gas-phase tracer experiment has been conducted in the lysimeter to help characterize the hydraulic and transport parameters of the soil. This facility will allow us to conduct very well-controlled experiments to examine the performance of the partitioning tracer method at the intermediate scale.

Mathematical Modeling

In preparation for the STOMP simulator to model the behavior of tracers in subsurface systems with NAPL, the performance of the simulator to compute multiple-phase flow through subsurface environments was improved for conditions of nonwetting fluid entrapment. The original version of the STOMP simulator modeled nonwetting fluid entrapment and scanning path hysteresis using the relative permeability-saturation-capillary pressure (k-s-p) theory developed by Lenhard and Parker (1987 Water Resources Research). This model, while shown to be accurate against a variety of laboratory experiments, was numerically inefficient and prohibited the dissolution or mobilization of nonwetting fluids (e.g., the dissolution and mobilization of entrapped NAPL by the aqueous phase). Simulations using this model were typicalIy limited to one-dimensional columns because of the excessive execution times caused by numerical instabilities resulting from the k-s-p theory implementation. Since the development of the Lenhard and Parker k-s-p theory and numerical model, Kaluarachichi and Parker developed a simplified k-s-p model for oil entrapment. This new theory is predicated on the assumption that hysteresis in wetting and drainage scanning paths is primarily due to the entrapment of nonwetting fluids and that the hysteresis due to contact angles and differences in pore-scale fluid entry and drainage pressures could be ignored. This simplification has impacts beyond those first suggested by Kaluarachichi and Parker of reducing the computational effort and storage requirements of implementing the k-s-p model. Their simplified model additionally allows dissolution and mobilization of entrapped nonwetting fluids because the wetting path reversal point is singular and directly related to the free and entrapped fluid saturations and is no longer dependent on the path histories. This feature additionally allows the specification of initial entrapped fluid quantities without having to create saturation path histories for each node point. This simplified model of Kaluarachichi and Parker, including air entrapment for three-phase eases, has been incorporated into the Water-Air and Water-Oil-Air operational modes of the STOMP simulator and is currently been verified for proper execution.