Environmental Management Science Program

Project ID Number 55216

In-Situ Characterization of Dense Non-Aqueous Phase Liquids Using Partitioning Tracers

Gary A. Pope
University of Texas at Austin
CPE 2.502
Austin, Texas 78712
Phone: 512-471-3235
E-mail: Gary_Pope@pe.utexas.edu

June 1, 1998

In-Situ Characterization of Dense Non-Aqueous Phase Liquids Using Partitioning Tracers

Gary A. Pope, University of Texas at Austin

Research Objective

Major advances have been made during the past year in our research on interwell partitioning tracer tests (PITTs). These advances include: (1) progress on the inverse problem of how to estimate the three-dimensional distribution of NAPL in aquifers from the tracer data, (2) the first ever partitioning tracer experiments in dual porosity media, (3) the first modeling of partitioning tracers in dual porosity media, (4) experiments with complex NAPLs such as coal tar, (5) the development of an accurate and simple method to predict partition coefficients using the equivalent alkane carbon number approach, (6) partitioning tracer experiments in large model aquifers with permeability layers, (7) the first ever analysis of partitioning tracer data to estimate the change in composition of a NAPL before and after remediation, (8) the first ever analysis of partitioning tracer data after a field demonstration of surfactant foam to remediate NAPL, and (9) experiments at elevated temperatures.

Research Progress and Implications

Inversion of Tracer Data: We have developed a new analytic approach that has several advantages over existing approaches for inversion of tracer data. First, the technique utilizes an extremely efficient three-dimensional multiphase streamline simulator as a forward model. Second, the parameter sensitivities are formulated in terms of one-dimensional integrals of analytic functions along the streamlines. Thus, the computation of sensitivities for all model parameters requires only a single simulation run to construct the velocity field and generate the streamlines. The inversion of tracer data is then performed using a two-step iterative linearization that involves first 'lining-up' the breakthrough times at the producing wells and then matching the production history. Our approach follows from an analogy between streamlines and ray tracing in seismology. The inverse method is analogous to seismic waveform inversion and thus, allows us to utilize efficient methods from geophysical imaging. The new approach has been applied for estimating permeability distribution based on conservative tracer tests (D.W. Vasco and A. Datta-Gupta: "Asymptotic Solutions for Solute Transport: A Formalism for Tracer Tomography," Submitted to Water Resources Research, December 1997), and is currently being extended for analysis of partitioning tracer data.

In estimation of spatially distributed parameters such as permeability and DNAPL saturation, it has been recognized for a long time that data is never abundant enough to constraint the parameters uniquely. The new approach taken in this research is to recognize this fact from the beginning and to solve for an ensemble of solutions, each equally valid. The nonuniqueness issue is attacked from different perspectives. First, Genetic Algorithms (GAs), an efficient optimization search method, are used. GAs span the whole search space, act as a directed Monte-Carlo search and produces the initial set of valid solutions. Each solution is then refined using a classical gradient-based method. Second, the solutions are forced to be smooth in some sense by adding a penalty term to the objective function. Solutions showing unnatural variations of parameter values are thus penalized. Third, a cluster analysis is used to group together similar solutions. Characterization of the uncertainty of the solution, often overlooked, is treated fully through two approaches. They both involve the computation of the sensitivity matrix but extract different information from it. This approach is currently being tested on both realistic synthetic examples and field data from the saturated PITTs at Hill AFB and the unsaturated PITTs at Kirtland AFB.

Dual porosity media: The first ever partitioning tracer experiments were completed in dual-porosity rock. These studies are needed to understand the behavior of partitioning tracers in

such media, to compare with flow and transport models, to select the best tracers and operating conditions, and ultimately to determine the viability and applicability of partitioning tracer technology for characterizing nonaqueous phase liquid contamination in dual-porosity aquifers. The first experiment was done in a Berea sandstone with a single fracture with and without NAPL in the fracture. Figure 1 shows the separation of the nonpartitioning (IPA) and partitioning (n-heptanol) tracer response curves for one of the experiments with residual NAPL (decane) in the fracture. The results of these experiments clearly show the combined impacts of partitioning to the NAPL, fracture transport and matrix diffusion. To the best of our knowledge, no such experiments have been reported in the literature, so the experimental methodology, partitioning tracer technology and interpretation approach are all entirely new and must continue to be developed. A variety of other tracers with different diffusion coefficients and partition coefficients have been tested to start this process. An analytical model was used to interpret these partitioning tracer single-fracture studies. The model shows very good agreement with the laboratory results. The agreement indicates that the physical processes assumed in the model are similar to the actual processes occurring in the laboratory experiments. The understanding of these processes that we have gained is essential to continued development of partitioning tracer technology as applied to fractured aquifers. The first ever field scale modeling is under way using UTCHEM, a simulator which includes the necessary features for modeling both tracer partitioning and dual-porosity tracer transport. These simulations are essential for our understanding of the relative importance of various parameters and characteristics for partitioning tracer test design in fractured media. Inspectional analysis has been used to determine the appropriate nondimensional scaling groups to aid in the understanding and generalization of our studies with fractured media.

Figure 1: Dual-porosity experiment showing nonpartitioning and partitioning tracers

Compositional analysis: Two vadose zone partitioning interwell tracer tests were completed at Kirtland Air Force Base to evaluate a radio frequency enhanced soil vapor extraction remediation technology. The remediation effort was a project of the Advanced Applied Technology Demonstration Facility. This effort was the first attempt to estimate the change in the composition of the NAPL after remediation. The Peng-Robinson equation-of-state was used to model the thermodynamic interaction between the hydrocarbons and the partitioning tracers. From this interaction, the compositional effects were determined. The results are unique in that they give not only the volume of NAPL removed, but also the change in composition due to the remedial action. This work is relevant to the many field sites where the NAPL consists of a complex chemical mixture and where the remediation process causes large changes in its composition.

Complex NAPLs: Alcohol tracer partition coefficients for coal tar have been measured and are compared to similar values for several different NAPLs in Figure 2. Coal tar is a multicomponent dense, nonaqueous phase liquid (DNAPL) primarily composed of polycyclic aromatic hydrocarbons. Despite the great complexity of coal tar, the results in Figure 2 show that the partition coefficients

can be predicted using the equivalent alkane carbon number approach just as well as for simple NAPLs such as trichloroethylene and decane. We have also investigated other very complex NAPLs such as a fuel oil with very high viscosity and in all cases we have found that the equivalent alkane carbon number approach is useful for correlating the tracer partition coefficients.

Figure 2. Comparison of predicted and measured partition coefficients of various alcohol tracers with various NAPLs.

Planned Activities

Not Provided