ANNUAL REPORT FOR ENVIRONMENTAL MANAGEMENT SCIENCE PROGRAM PROJECT NUMBER 86598 COUPLED FLOW AND REACTIVITY IN VARIABLY SATURATED POROUS MEDIA

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RESEARCH OBJECTIVE

Improved models of contaminant migration in heterogeneous, variably saturated porous media are required to better define the long-term stewardship requirements for U.S. Department of Energy (DOE) lands and to assist in the design of effective vadose-zone barriers to contaminant migrations. The objective of our three-year project is to meet the DOE need by developing new experimental approaches to describe adsorption and transport of contaminants in heterogeneous, variably saturated media (i.e., the vadose zone). The research specifically addresses the behavior of strontium, a high priority DOE contaminant. However, the key benefit of this research is improved conceptual models of how all contaminants migrate through heterogeneous, variably-saturated, porous media. Research activities are driven by the hypothesis that the reactivity of variably saturated porous media is dependent on the moisture content of the medium and can be represented by a relatively simple function applicable over a range of scales, contaminants, and media. A key and novel aspect of our research is the use of the 2-meter radius geocentrifuge capabilities at the Idaho National Laboratory (INL) to conduct unsaturated reactive transport experiments (Figure 1). The experimental approach using the geocentrifuge provides data in a much shorter time period than conventional methods allowing us to complete more experiments and explore a wider range of moisture contents. The vadose zone research being done in this project will demonstrate the utility of environmental geocentrifuge experimental approaches and their applicability to DOE's vadose research needs.

Figure 1. INL geocentrifuge with experimental box mounted on the platform.

RESEARCH PROGRESS AND IMPLICATIONS

The objectives are being accomplished by conducting integrated conventional laboratory column experiments and geocentrifuge approaches to assess breakthrough curves for one- and two-dimensional systems with constructed heterogeneities under conditions of variable moisture content. In addition, we plan to conduct similar experiments using intact cores of natural soil formations. This report summarizes our progress as of September, 2005 and represents the first 2.5 years of a three-year project. Key activities to date are described in the following paragraphs.

Review of the theory of unsaturated flow in the geocentrifuge. We have derived an expression for fluid potential that includes both centrifugal and gravitational accelerations. This equation was derived from the Navier-Stokes equation as well as from energy balance equations. From this expression of fluid potential and the relationship between pressure and the height of the water column in a piezometer, equations for the specific discharge are obtained in terms of pressure, pressure head, and hydraulic head for both fixed arm and swinging bucket centrifuges. The centrifugal component of the specific discharge written in terms of hydraulic head involves a term of $\partial\left(h^2\right)/\partial r$ rather than $\partial h/\partial r$.

These results suggest that previously proposed scaling models be reconsidered or that at least qualifying criteria be applied. We show from the Navier-Stokes equations applied to porous media flows within a geocentrifuge the relative effects that a variable gravity field, represented by the centrifugal force and the coriolis force, have on the flow fields. Nondimensionalization of the governing equations shows the role that the Ekman and Rossby numbers play in these porous media flows. This analysis provides information useful for the scaling of variable gravity geocentrifuge experiments and helps to define the theoretical limits under which geocentrifuge experiments exhibit similarity to field phenomena. We will present our revised and expanded theory at the National Meeting of the Geological Society of America in Salt Lake City, UT, October, 2005.

Development of numerical tools. We are collaborating with Dr. Jirka Simunek to modify the Hydrus 1D and Hydrus 2D codes to account for variable acceleration encountered on the centrifuge. We are using these codes to design of our experiments as well to analyze and interpret our experiments. In addition, Dr. Simunek has provided a modified code that will allow us to include the dependence of the reactivity on the water saturation. Simulations of solute transport in variably saturated media with this dependence of reactivity have been completed and are being written up as part of a manuscript to be submitted in the next 3 weeks.

Design and construction of an in-flight fraction collector. While sample collection is well established for conventional laboratory experiments, there is little experience in identifying robust instrumentation that can be remotely controlled while in flight on the geocentrifuge. We have designed and constructed a vacuum operated fraction collection system that can be controlled in-flight. The current design will allow us to collect up to 26 samples of up to 10 ml each. The system can be easily cascaded to yield more samples if needed.

Design, construction, and calibration of soil moisture sensors. In-flight soil moisture measurements are required for studies of transport in unsaturated porous media. We have modified the design of the commercially available ECH_2O probes for measuring soil moisture content. The new design consists of a flexible electrode that is affixed to the inside wall of circumference. Calibration of the electrodes suggests that water saturation can be measured to within ±3% over the range of 0 to 100% saturation. A manuscript is being revised for the Vadose Zone Journal.

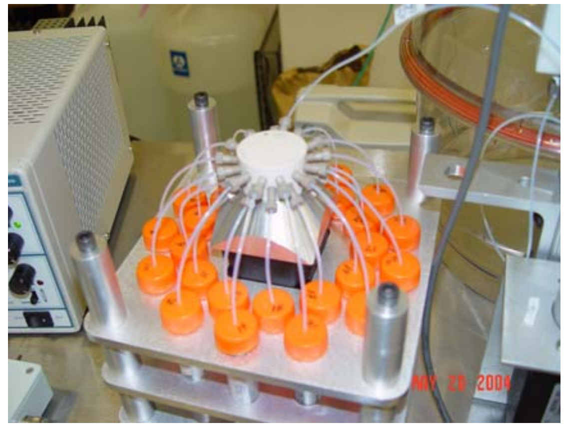

Figure 2. Fraction collector for geocentrifuge experiments.

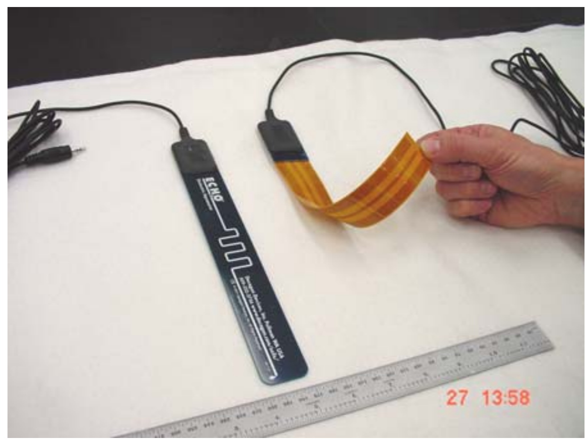

Figure 3. Original design of ECH2O probe (left) and new flexible design (right).

Falling head tests in the geocentrifuge. To test some of our theories on flow through porous media in a centrifugal field and to provide a tool for rapidly determining saturated hydraulic conductivity of our soils, we conducted falling head tests at 1, 10, 20, and 30 g. While the test conducted a 1 g follows conventional theory of a linear relationship between the log of hydraulic head and time, the other tests significantly deviate from this linear behavior Figure 4. This result is contrary to assumptions in the published literature. Based on our previously described theoretical development of the equations of flow in a centrifugal field, we are currently deriving equations describing falling head test data on the geocentrifuge.

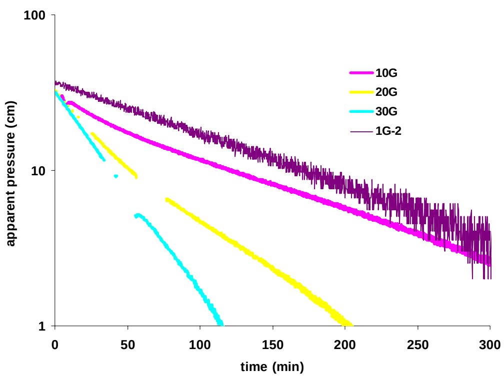

Figure 4. Hydraulic head versus time for falling head tests run at 1 g and on the geocentrifuges at 10, 20 and 30 g.

Breakthrough curves. Experimental break through curves (BTCs) of a conservative tracer were obtained on a 30-cm long column to test fluid delivery systems and general design concepts. At the top of the column, a constant flux of water was established over a porous plate to provide a uniform flow field. A constant pressure condition was established at the bottom of the column using a porous membrane and a vacuum system. An electrical conductivity (EC) probe provided real-time monitoring of the tracer in the outflow at one-second intervals. Solute BTCs were obtained at 10 to 40 g acceleration. The time it takes to obtain a BTC varies with the inverse of the acceleration. These curves were obtained in approximately $1/N^{th}$ of the time it takes by conventional techniques where N is the centrifugal acceleration in g. The dispersion in the BTCs increases with increasing N.

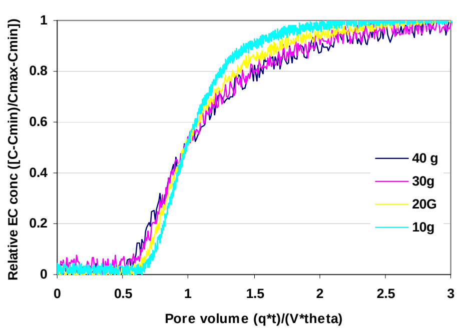

Figure 5. EC breakthrough curves obtained from one-dimensional column on the geocentrifuge

Centrifuge Upgrade. We have upgraded the communication system between the experimental control computer on the geocentrifuge to the computer in the geocentrifuge control room. The INL centrifuge was originally purchased with a fiber optic rotating joint/electric slip ring assembly to transmit data from computers on the centrifuge to computers in control room. We have now removed this rotating joint/slip ring assemble and replace it with a wireless ethernet and video system. In typical geotechnical experiments, the centrifuge is only operated for a period of minutes to a few hours. Although we can greatly speed up the time to complete a solute transport experiments in unsaturated soils using the geocentrifuge, these experiments still require operation periods that can take up to a number of days. We found that our fiber optic/slip ring assembly was not robust enough to handle these long run time and have now upgraded to wireless transmission technology.

PLANNED ACTIVITIES

We will begin our one-dimensional reactive transport experiments on ostensibly homogeneous systems to determine the properties of the materials that will be used in the two-dimensional experiments that will be conducted later. In addition, conventional column experiments using a vacuum chamber will provide comparison between techniques. Both types of experiments will utilize conservative (Cl^-) and reactive tracers (Sr^{2+}, Zn^{2+}, F^-) to obtain BTCs as functions of moisture content. In addition, moisture content-matric potential- hydraulic conductivity relationships will be experimentally obtained. Our experimental results will be used to determine reactivity-moisture content relationships.

Two-dimensional tracer experiments will be conducted using the geocentrifuge using obviously heterogeneous materials. The type of heterogeneities will include: 1) systems with continuous alternating horizontal layers of low and high permeability; 2) systems with continuous alternating vertical bands of low and high permeability that can simulate vertical fractures (INEEL) or clastic dikes (Hanford); and 3) systems with discontinuous high permeability layers in a low permeability matrix or discontinuous low permeability layers in a high permeability matrix that simulate clay lenses or the current conceptualization of the INEEL vadose zone. Although the experiments examine idealized-heterogeneity, the heterogeneity patterns capture the essential features and characteristics of common types of heterogeneities observed at DOE sites.

INFORMATION ACCESS

Discussions of our project were presented at the Geocentrifuge Workshop held at the Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID, March 27-28, 2003. Information about the workshop and summaries of presentations can be found at www.inel.gov and under “geocentrifuge”.

Dr. E.D. Mattson gave a presentation the Southern Idaho Section ASCE on October 23 on Environmental and Geo-Engineering Research at the INEEL focused on our geocentrifuge studies.

A poster session of geocentrifuge techniques at the annual American Geophysical Union meeting in San Francisco was organized by Drs. E.D. Mattson (INEEL) and P. Culligan (Columbia University). We were associated with five posters at the session.

Project presentations and posters include:

Nakajima, H., E.D. Mattson, and A.T. Stadler, 2004. "Application of Geotechnical Centrifuge to Determine Unsaturated Soil Parameters." 57th Canadian Geotechnical Conference. October 24-26. Quebec Canada.

Palmer, C.D., J. Crepeau, R.W. Smith, E.D. Mattson, 2005. Fluid flow through porous media in a centrifugal field. Geological Society of America Annual Meeting. October 16-19, 2005, Salt Lake City, UT.

Palmer, C.D., E.D. Mattson, K. Baker, R.W. Smith, 2004. Geocentrifuge Applications to Solute Transport in the Vadose Zone. Geological Society of America Annual Meeting. November 8-10, 2004, Denver, CO.

Palmer, C.D., E.D. Mattson, and R.W. Smith Coupled flow and reactivity in variably saturated porous media. EMSP Annual PI meeting, May 6-7, 2003, EMSL Facility, Richland, WA. (See www.pnl.gov/emsp/fy2003/presentations/palmer_carl_86598.pdf).

Mattson, E.D., K.E. Baker, C.D. Palmer, R.W. Smith, and J. Simunek, 2003. One-dimensional solute transport in variably saturated soil using a geocentrifuge apparatus. American Geophysical Union Meeting, San Francisco, CA, Dec. 8-12, 2003.

Simunek, J., E.D. Mattson, and C.D. Palmer, 2003. Modifications of the HYDRUS software packages for analyzing transient flow and solute transport experiments from the centrifuge. American Geophysical Union Meeting, San Francisco, CA, December 8-12, 2003.

C.D. Palmer, J. Crepeau, R.W. Smith, 2003. Fundamental equations of flow in the geocentrifuge. American Geophysical Union Meeting, San Francisco, CA, December 8-12, 2003.

Nakajima, H., E.D. Mattson, and A.T. Stadler. Unsaturated hydraulic properties determined from geocentrifuge tests. American Geophysical Union Meeting, San Francisco, CA, December 8-12, 2003.

R.M. Holt, R.J. Glass, J.M. Sigda, and E.D. Mattson. Phase structure in a dentrifugal field: Impact of capillary heterogeneity and angular velocity. American Geophysical Union Meeting, San Francisco, CA, December 8-12, 2003.

Manuscripts include:

E.D. Mattson, K.E. Baker, and C.D. Palmer, C.R. Breckenridge, J. Svoboda, R.W. Smith,. A Flexible Moisture Content Probe for Unsaturated Soil Column Experiments. Being revised.

Palmer, C.D., J. Crepeau, R.W. Smith, E.D. Mattson. Equations of flow through porous media in a centrifugal field. Being reviewed.

R.W. Smith, C.D. Palmer, E.D. Mattson. Dependence of retardation factors on soil moisture content. Draft.