CONF-9005117--5

Received by OSTI
APR 19 1990

SAND89-2359C

LABORATORY RESEARCH PROGRAM TO AID IN DEVELOPING AND TESTING THE VALIDITY OF CONCEPTUAL MODELS FOR FLOW AND TRANSPORT THROUGH UNSATURATED POROUS MEDIA*

R.J. Glass
Geoscience Analysis Division, 6315
Sandia National Laboratories
Albuquerque, NM, USA

SAND--89-2359C

DE90 009532

ABSTRACT

As part of the Yucca Mountain Project, a laboratory research program is being developed at Sandia National Laboratories that will integrate fundamental physical experimentation with conceptual model formulation and mathematical modeling and aid in subsequent model validation for unsaturated zone water and contaminant transport. Experimental systems are being developed to explore flow and transport processes and assumptions of fundamental importance to various conceptual models. Experimentation will run concurrently in two types of systems: fractured and nonfractured tuffaceous systems; and analogue systems having specific characteristics of the tuff systems but designed to maximize experimental control and resolution of data measurement. Questions to which experimentation currently is directed include infiltration flow instability, water and solute movement in unsaturated fractures, fracture-matrix interaction, and the definition of effective large-scale properties for heterogeneous, fractured media.

*This work was performed under the auspices of the U.S. Department of Energy, Office of Civilian Radioactive Waste Management, Yucca Mountain Project, under contract DE-AC04-76DP00789. This document was prepared under Quality Assurance Level III and WBS 1.2.1.4.6.

INTRODUCTION

The U.S. Department of Energy is investigating a prospective site for a high-level nuclear waste repository located in unsaturated volcanic ash (tuff) deposits hundreds of meters above the water table at Yucca Mountain, Nevada. As part of this investigation, the ability of the natural system to restrict water movement and to retard the migration of radionuclides if released must be assessed. While this assessment will be made with respect to specific regulations formulated by the U.S. Nuclear Regulatory Commission and Environmental Protection Agency, it must be made with a sound scientific understanding of the flow and transport processes that occur at the site. Because there always will be uncertainty with respect to the processes occurring, our modeling of these processes, and the temporal and spatial distribution of model parameters, the final analysis will have to be cast in terms of probability. To develop this general understanding, we must systematically

1) identify all processes by which radionuclides could migrate through the rock formation to the biosphere;
2) develop basic scientific understanding of these processes through fundamental conceptual and mathematical modeling, controlled experimentation, and model validation (invalidation) exercises;
3) bound the occurrence of various processes in terms of system parameters such as initial conditions, boundary conditions, and distribution of properties (in both time and space) that must be present; and
4) pose informational needs for site characterization so that the probability of occurrence for each process may be assessed, and appropriate model parameters measured.

Fundamental questions concerning flow and transport in unsaturated porous media can be addressed through controlled laboratory experimentation. A laboratory research program is being developed at Sandia National Laboratories for the Yucca Mountain Project that will integrate fundamental physical experimentation with conceptual model formulation and mathematical modeling and aid in testing the validity of models at the meter scale. The laboratory program is part of a broader effort currently being planned that will address the validity of conceptual models used in calculation of groundwater travel time and radionuclide transport through the unsaturated zone at Yucca Mountain. Questions raised in thought experiments and field studies will be used to direct laboratory experimentation. In general, research in the laboratory is prioritized with respect to understanding flow processes which could cause the site to fail to meet regulatory requirements (i.e., decrease water or radionuclide travel time), the testing of key assumptions in models for processes considered to be important, and the development of new conceptual models as found to be necessary. The research program stresses fundamental research and in this sense will have broad applicability within the general field of flow and transport through unsaturated porous media.

In this paper, the laboratory research program is outlined. The general approach for laboratory experimentation will be presented followed by an outline of several areas of research where studies are currently underway. The program is designed to be flexible. Future studies will be defined as the broader validation effort develops and key informational needs are determined that require a further understanding of flow and transport mechanisms.

APPROACH AND METHODS FOR LABORATORY RESEARCH PROGRAM

Laboratory studies fill a critical need to test our understanding of basic processes. Simple qualitative experimentation with the goal of demonstrating a process is necessary as a first step toward understanding. Fundamental understanding, however, comes through systematic quantitative experimentation, conceptual modeling, and model validation exercises. The approach for the laboratory research program is directed to achieve fundamental understanding.

Two types of experimental systems will be used. The first is in tuffaceous systems and thus contains all the natural complexity of the rock. Rock types will vary from bedded nonwelded to nonbedded nonwelded, partially welded and welded tuff with and without fractures. Experimental samples will be taken from either Yucca Mountain or natural analogue sites. The second type of experimental system is analogous to the tuff system but simpler, having only certain predetermined attributes of the tuff. These analogue systems are designed to maximize experimental control (i.e., ability to systematically vary system parameters) and resolution of data measurement. To allow systematic variation of hydraulic properties, the analogue systems will be composed of unconsolidated sand, glass beads, porous glass beads, or "rocks" fabricated to specification (e.g., ceramics, sintered glass, or sintered metal). Rough-walled fractures will be simulated with roughened glass plates or fabricated rocks held together at different spacings. Experimentation in both types of systems will run concurrently, with experimentation in analogues driven by what we know about or discover from work in tuff systems and vise versa.

The experimental systems also will strive to acquire high-resolution temporal and spatial data to allow the possibility of identification of additional flow and transport mechanisms. For questions requiring full three-dimensional data acquisition, tomographic techniques using either x-ray or gamma-ray transmission, nuclear magnetic resonance, positron emission or other methods will be developed and applied. Most of these methods, however, are limited in the size of system to which they can be applied. For many of the questions we are currently investigating, experiments on the scale of a meter are required. To obtain high quality data at the meter-scale, two-dimensional experiments are conducted in extensive (1x1m) but thin (0.01m) slabs of material. Data measurement techniques for thin slabs include optical, x-ray, and gamma-ray transmission techniques. For many experiments we will concentrate on the first two as they are rapid and can be used as "field" measurement techniques while the gamma-ray densitometer is much slower and is primarily a point measurement technique.

Analogue systems will be designed to take full advantage of optical techniques. Optical techniques for visualizing moisture content make use of the fact that transmission of light through translucent media, such as silica sand or glass beads, increases with an increase in moisture content. By illuminating the back of a thin slab of media, the moisture content integrated over the thickness of the slab is visualized as light intensity that varies from point to point at the front of the slab. Intensity fields can be recorded up to 30 times a second and digitized into an array of 512 x 512 or more points using video imaging technology. Currently the optical technique is being used qualitatively to determine "relative" moisture content (one location is wetter or drier relative to another). To further develop the technique, we are developing calibration methods and comparing the optical technique with a standard gamma-ray densitometer. An adaption of the technique will also be used to visualize transient dye concentration in steady state flow fields. Calibration methods to allow quantitative measurement of concentration are currently in development. Preliminary results indicate the optical technique is also useful in visualizing packing-induced heterogeneity and thus it may be possible to use it to characterize heterogeneity as well.

For opaque tuffaceous systems, x-rays replace light and their attenuation is used to measure moisture content in extensive thin slabs. X-ray fluorescing film placed on the back side of the slab transforms the x-ray intensity field into a visible light intensity field which again is visualized, recorded, and digitized using video imaging technology. For situations that do not require high spatial and temporal resolution, a standard gamma-ray densitometer is used.

In experimental design, concepts of nondimensionalization, scaling, and similarity are developed and applied to increase understanding and generalize results [1, 2, 3, 4]. For systems where these concepts are applicable, once a physical experiment is conducted or a solution of the dimensionless form of the governing equation has been calculated for one porous medium, the results apply immediately to all similar porous media and flow systems through scaling relations. Systematic exploration of dimensionless parameter space allows the efficient characterization of system response for all possibilities of the dimensional parameters. The concept of similar porous media can also be exploited to allow experimentation in porous media similar to the one of primary interest. This can minimize the experimental difficulties of working with some porous materials where the time scale of the flow process is either too short or too long to make measurement practical.

CURRENT STUDIES

A number of studies, in various stages of planning or completion, are underway to aid in the development of the laboratory research program. These studies are being used not only to develop techniques and train personnel but to increase our understanding of several identified flow processes and to challenge several key assumptions embodied in many currently accepted conceptual models. The studies can be grouped into four main areas of research: infiltration flow instability; water and solute movement in unsaturated fractures; fracture/matrix interaction; and the definition of effective large-scale properties for heterogeneous, fractured media.

1) Infiltration flow instability

Most conceptual models assume that infiltration flows are essentially stable with any irregularity in the flow field caused by spatial variability in hydraulic properties, initial conditions, or boundary conditions. Yet, gravity-driven instability of an infiltration flow or "wetting front instability" can cause the flat wetting front moving downward through an unsaturated porous medium to break into fingers which move vertically, bypassing a large portion of the vadose zone. Wetting front instability within porous media has been demonstrated in both laboratory and field settings and has been shown to have a dramatic effect on water and solute transport [5, 6, 7, 8, 9]. The development of a two zone moisture content field consisting of high moisture content finger cores surrounded by lower moisture content fringe regions and the persistence of this structure from infiltration cycle to infiltration cycle has also been demonstrated and explained with a simple theory based on hysteresis in the moisture characteristic relations [10]. The dependence of finger properties on system parameters for initially dry, coarse, narrow grain size distribution sand has been determined through dimensional analysis and experimentation [11, 12]. Stability criteria and relations for finger width or diameter have also been formulated through linear stability analysis and compared to experimental data showing remarkable agreement for homogeneous media where the analysis applies [13, 12].

Generalization of the results obtained from these previous theoretical and experimental studies suggests many situations, such as an increase in conductivity with depth, unsaturated infiltration from a boundary held at less than saturation, and redistribution following an infiltration event, can cause a wetting front to become unstable and persistent fingers to form. Since all of these situations occur at Yucca Mountain, the process of wetting front instability must be understood and bounded. To accomplish this, several complicating factors that may stabilize most situations must be explored. The most important of these factors are pore size distribution, contact angle (wettability), heterogeneity, and initial moisture content. A series of experiments to investigate the effects of these factors is currently underway in an extensive slab chamber using optical techniques to follow the evolution of the moisture content fields in silica sands. The grain size distribution of the sand and thus the pore size distribution of the media are being varied systematically. Similarity theory applied to finger properties is used to design the grain size distributions investigated. Thus the ability of similarity theory to predict finger properties (width and velocity) will also be tested. Several preliminary experiments in horizontally microlayered sand systems suggest that fingers widen and perhaps are suppressed as the amplitude of the property oscillation between layers and spatial frequency increase. A series of experiments where microlayering is systematically varied is planned as are experiments where the effects of contact angle and initial moisture content will be systematically explored.

Invasion percolation theory modified to include contact angle, buoyancy, multiple neck pore filling facilitation, and initial moisture content is being used to build a conceptual model which incorporates the essentials of the pore scale mechanism for finger formation. Combination of experimentation and modeling should allow the bounding of gravity-driven fingering in porous media and thus the ability to assess its occurrence at Yucca Mountain. Our current work investigating flow through rough-walled fractures (2 below) has demonstrated that gravity driven fingers occur in vertical simulated fractures as well.

2) Water and solute movement in unsaturated fractures

Many of the units of tuff composing both the saturated and unsaturated zones at Yucca Mountain are considered to be highly fractured [14]. Therefore an understanding of the effects of fractures on water and solute transport within these zones is crucial. In the extreme of very low permeability matrix such as in highly welded, vitric tuff, or for matrix which is near saturation, the effect of the matrix on flow and transport through a conducting fracture will be of second order. As a first step toward understanding the more difficult problem where the influence of the matrix on flow through the fracture cannot be neglected, we will study unsaturated flow within a fracture in impermeable media.

Little is known concerning the distribution of water and air in an unsaturated fracture and its influence on flow and transport through the fracture. In both analogue and welded tuff systems the effects of fracture surface roughness and orientation in the gravity field on unsaturated fracture flow field structure and solute transport will be studied systematically. In particular, gravity-driven instability causing the formation of downward-moving fingers within the fracture should be present in nonhorizontal unsaturated fractures. Preliminary analogue systems consist of two roughened glass plates held together to form a simulated fracture. Six different roughnesses are being used, and the angle of the fracture plane with respect to gravity is varied. The structure of transient and steady state flow fields in the glass fractures is recorded photographically or on video and analyzed using digital image analysis. The use of dye pulses in the water supplied to the fracture may allow the characterization of solute transport through these systems as well and will be explored in future studies. Subsequent studies will also be made in molds of natural fractures, natural fractures in welded tuff, and fabricated, fractally generated fractures machined into surfaces.

3) Fracture-matrix interaction studies

In fractured, permeable rock formations, the movement of water and solutes between fractures and porous matrix (fracture-matrix interaction) can have a profound influence on the rate at which water and solutes will migrate through the formation. Models of flow through fractured rocks are based on assumptions concerning the fluid and solute transfer between fractures and adjacent porous matrix. Basic research will be performed to understand fracture-matrix interaction (for both water and solute) and challenge our current assumptions concerning the process.

The influence of flow field structure in unsaturated fractures which distribute water nonuniformly within a fracture, on fracture-matrix interaction will be studied. The influence of gravity-driven instability to cause fingers within a fracture which may persist and greatly influence fracture-matrix interaction will be considered. We will begin with a simulated fracture one side of which will be impermeable and clear (glass) and the other side will be porous (ceramic, sintered glass beads or ground tuff). Such a system will allow us to document carefully the structure of water contained in the fracture while tensiometers installed in the porous side will monitor the transient pressure field.

The physics of fluid and dissolved contaminant transfer between a fracture and the surrounding porous matrix in the presence of a fracture coating or alteration zone will also be explored. Porous media composing the matrix will be fabricated by sintering packs of glass beads. After homogeneous matrix blocks have been made, material will be added to a side of the block to constitute a coating. The thickness of the coating material and its properties will be varied. The permeability and porosity of the coating material will be measured using standard techniques on larger homogeneous blocks made from the same material. To understand altered surface chemical properties of a fracture coating requires the systematic variation of the surface chemical properties. Technology exists to alter the surface properties of glass through a number of processes developed for chromatographic analysis of chemical solutions. These techniques may be applied to the fabricated coating layers to allow a systematic exploration of geochemical processes.

4) Definition of effective large-scale hydraulic properties for heterogeneous, fractured media

Experimentation and subsequent modeling of water movement in a small unsaturated core of tuff have shown the matrix properties of tuff to be highly variable on the centimeter scale [15, 16]. In addition, fractures and microfractures are present in many tuff formations. The definition of equivalent or effective properties on the scale of a meter or greater which embody these smaller scale heterogeneities is essential for repository-scale calculations of water and radionuclide transport. To aid in the formulation and testing of equivalent media property models we will conduct experimental studies in both analogue and tuff systems.

In analogue systems, porous media with different heterogeneity structure and with and without high permeability fractures will be generated in sand and fabricated rock material. Transient infiltration experiments will be conducted in extensive slab systems composed of these materials and the moisture content within the flow field will be recorded in time using either optical or x-ray techniques and video/digital imaging. Boundary conditions around the edge of the slab will be controlled using porous pressure plates to supply either known pressure or flux. Steady state moisture flow with transient solute transport experiments will also be conducted. Data will allow the evaluation of equivalent porous media concepts in well parameterized systems.

In tuff systems, thin slabs of tuff up to 1 m square will be cut and ground smooth. Impermeable material will be contact cemented to the sides of the slabs and porous pressure plates will be installed around the edges of the slabs to impose known boundary conditions. Since most slabs will contain naturally occurring fractures, their influence on the developing flow field can be evaluated. Transient infiltration experiments will be conducted and moisture contents within the flow field will be recorded in time using x-ray techniques and video/digital imaging. By cutting slabs along the principal axes of visual bedding and supplying water to a small hole in the center of the slab, anisotropy on the scale of the experiment can be evaluated. Transient solute transport experiments will also be conducted using x-ray absorbing solute or radioactive tracers.

CONCLUSION

Conceptual models applied to predict long-term transport of water and radionuclides at Yucca Mountain or elsewhere must be evaluated critically to test their validity. Conceptual model formulation begins by making simplifying assumptions. For a model to accurately predict physical system response, the physics of the major processes that occur for the range of parameter space, physical scale and boundary conditions within which the model will be applied must be represented adequately. The goal of the laboratory research program being developed at Sandia National Laboratories is to acquire the fundamental scientific understanding of flow and transport processes that may occur in the unsaturated zone at Yucca Mountain and thereby assist in developing and testing the validity of our conceptual models.

REFERENCES

Miller, E.E., and R.D. Miller : "Physical theory for capillary flow phenomena", J. Appl. Phys. (1956) 27:324-332.

Kline, S.J. : Similitude and Approximation Theory. McGraw-Hill Inc., New York, 1965.

Tillotson P.M. and D.M. Nielsen : "Scale factors in soil science", Soil Sci. Soc. Am. J. (1984) 48:953-959.

Sposito, G., and W.A. Jury : "Inspectional analysis in the theory of water flow through unsaturated soil", Soil Sci. Soc. Am. J. (1985) 49:791-798.

Hill, D.E., and J.-Y. Parlange : "Wetting front instability in layered soils", Soil Sci. Soc. Am. Proc. (1972) 36:697-702.

Starr, J.L., H.C. DeRoo, C.R. Frink, and J.-Y. Parlange : "Leaching characteristics of a layered field soil", Soil Sci. Soc. Am. J. (1978) 42:376-391.

Glass, R.J., T.S. Steenhuis, G.H. Oosting, and J-Y Parlange : "Uncertainty in model calibration and validation for the convection-dispersion process in the layered vadose zone", Proc. Int. Conf. and Workshop on Validation of Flow and Transport Models for the Unsaturated Zone, Ruidoso, NM, 1988, 119-130.

Glass, R.J., T.S. Steenhuis, and J.-Y. Parlange : "Wetting front instability as a rapid and far-reaching hydrologic process in the vadose zone", J. of Contam. Hydrol. (1988) 3:207-226.

Glass, R.J., G.H. Oosting, and T.S. Steenhuis : "Preferential solute transport in layered homogeneous sands as a consequence of wetting front instability", J. of Hydrol. (1989) 110:87-105.

Glass, R.J., T.S. Steenhuis, and J.-Y. Parlange : "Mechanism for finger persistence in homogeneous unsaturated porous media: Theory and verification", Soil Sci. (1989) 148:60-70.

Glass, R.J., J.-Y. Parlange, and T.S. Steenhuis : "Wetting front instability I: Theoretical discussion and dimensional analysis", Water Resour. Res. (1989) 25:1187-1194.

Glass, R.J., T.S. Steenhuis, and J.-Y. Parlange : "Wetting front instability II: Experimental determination of relationships between system parameters and two dimensional unstable flow field behavior in initially dry porous media", Water Resour. Res. (1989) 25:1195-1207.

Parlange, J.-Y., and D.E. Hill : "Theoretical analysis of wetting front instability in soils", Soil Sci. (1976) 122:236-239.

Montazer, P., and W.E. Wilson : "Conceptual hydrologic model of flow in the unsaturated zone, Yucca Mountain, Nevada", USGS-WRI-84-4345, (1984) U.S. Geological Survey, Lakewood CO.

Reda, D.C. : "Influence of transverse microfractures on the imbibition of water into initially dry tuffaceous rock", Flow and Transport Through Unsaturated Fractured Rock, Geophysical Monograph 42, eds. D.D. Evans and T.J. Nicholson, American Geophysical Union, Washington DC, 1987, 83-90.

Eaton, R.R., and N.E. Bixler : "Analysis of a multiphase, porous-flow imbibition experiment in fractured volcanic tuff", Flow and Transport Through Unsaturated Fractured Rock, Geophysical Monograph 42, eds. D.D. Evans and T.J. Nicholson, American Geophysical Union, Washington DC, 1987, 91-98.

Appendix

Information from the Reference Information Base
Used in this Report

This report contains no information from the Reference Information Base.

Candidate Information
for the
Reference Information Base

This report contains no candidate information for the Reference Information Base.

Candidate Information
for the
Site & Engineering Properties Data Base

This report contains no candidate information for the Site and Engineering Properties Data Base.