

Project 0008673 - Advanced Conceptual Models for Unsaturated and Two-Phase Flow in Fractured Rock

Michael J. Nicholl - University of Idaho

Robert J. Glass - Sandia National Laboratories

Harihar Rajaram - University of Colorado

Thomas R. Wood - Idaho National Engineering and Environmental Laboratory

Research Objective: The Department of Energy Environmental Management Program is faced with two major issues involving two-phase flow in fractured rock; specifically, transport of dissolved contaminants in the Vadose Zone, and the fate of Dense Nonaqueous Phase Liquids (DNAPLs) below the water table. Conceptual models currently used to address these problems do not correctly include the influence of the fractures, thus leading to erroneous predictions. Recent work has shown that it is crucial to understand the topology, or 'structure' of the fluid phases (air/water or water/DNAPL) within the subsurface. It has also been shown that even under steady boundary conditions, the influence of fractures can lead to complex and dynamic phase structure that controls system behavior, with or without the presence of a porous rock matrix. Complicated phase structures within the fracture network can facilitate rapid transport, and lead to a sparsely populated and widespread distribution of concentrated contaminants; these qualities are highly difficult to describe with current conceptual models. The focus of our work is to improve predictive modeling through the development of advanced conceptual models for two-phase flow in fractured rock.

Research Approach: Preliminary experiments have shown that behavior at fracture intersections is key, thus we are employing systematic experimentation to identify and classify behavior at intersections. Understanding gained at the scale of individual fracture intersections will be used to augment a Modified Invasion Percolation Model (MIP) that has shown significant promise in predicting flow through fracture networks. Development of the MIP model will be iterative, in that we will use numerical simulations to design critical physical experiments at the network scale, which will challenge the model. The augmented, and fully tested MIP model will be exercised on realistic fracture networks for the purpose of understanding large-scale development of phase structure. Results of the large-scale network simulations will be abstracted to the data sets from the INEEL Vadose Zone Research Park so that critical features may be included in conceptual models used by the Environmental Management Science Program and the Idaho Closure Project.

Research Progress and Implications:

This project was initiated in FY03. As of June 1, 2004, we have accomplished the following:

- 1) Conducted a detailed evaluation of the preliminary experiments used to develop our investigative approach. In those experiments, water was invaded into an air-filled, two-dimensional analog fracture network at a variety of flow rates. Results demonstrated the critical control that fracture intersections place on two-phase flow in fracture networks. At low flows, capillary and gravitational forces combined to create a narrow pulsing flow structure that spanned the system vertically. At higher flows, viscous forces acted to remove the pulsation; however, the flow structure remained narrow. The intersections acted to impose a narrow "slender ladder" structure on the flowing phase that did not expand with depth, but instead remained focused. Results were published in *Water Resources Research* [Glass et al., 2003].
- 2) Initiated a collaborative relationship with a research group at Seoul National University. This group, which is led by Dr. Kang-Kun Lee is also using a combined experimental-numerical approach to consider DNAPL migration in fracture networks. They are particularly interested in the influence of ambient groundwater flows, making their work complementary to our interest in density-driven flows. The first fruit of that collaboration is an article demonstrating that modification of an Invasion Percolation algorithm to include gravity and the first-order effects of viscous forces shows good agreement with physical experiments in a simplistic fracture network. Results were published in *Geophysical Research Letters* [Ji et al., 2003a].
- 3) Conducted an extensive review of models for fracture networks. These include models developed from observations of networks on outcrops at several scales and stochastic models that are prevalent in the literature from the 1980s to very recent developments. The results of this review were included as part of a review paper co-authored by Rajaram, and published in *Reviews in Geophysics* [Molz et al., 2004].
- 4) Prepared a manuscript based on previous work that will be used to support the development of our new conceptual model(s) for transport in fractured rock. Eight experiments were conducted in a 2-D analog fracture-matrix network to evaluate the repeatability of flow under nearly identical conditions and to characterize general patterns in flow behavior. Data revealed that flow generally converged to a single fracture with depth. Periods of pathway switching were observed to be more common than periods with steady, constant flow pathways. We noted the importance of fracture intersections for integrating uniform flow and discharging a "fluid cascade", where water advances rapidly to the next capillary barrier, creating a stop and start advance of water through the network. The results of this simple experiment suggest that the interaction of multiple fracture intersections in a network creates flow behavior not generally recognized in popular conceptual and numerical models. Results were published in *Vadose Zone Journal* [Wood et al., 2004a].

5) Participated in the evaluation of a well completion technique developed by investigators at the INEEL (J.M. Hubbell, J.B. Sisson). Their design significantly reduces the deleterious effects of barometric fluctuations on water level measurements. Thus providing a means to more accurately predict water table gradients in fractured rock, such as is found at the INEEL. A manuscript co-authored by Nicholl was published in *Vadose Zone Journal* [Hubbell et al., 2004a].

6) Presented an overview of our project at the EMSP Principal Investigator Workshop in Richland, WA on May 6-7, 2003 [Nicholl et al., 2003].

7) A series of invited presentations regarding the experimental investigation of flow through unsaturated fracture networks were given by Nicholl at the following locations: North Dakota State University (1/31/03), Tufts University (2/11/03), University of Alabama (2/18/03), University of Massachusetts (3/10/03), University of California at San Diego (3/20/03), and University of Nevada at Las Vegas (3/28/03).

8) In collaboration with ongoing unsaturated fractured rock research at INEEL, we evaluated unit processes active at the scale of individual intersections that may explain dynamical behavior observed in experiments at the network scale (see 1 and 4 above). The competition between capillary, gravitational, viscous, and in some cases inertial forces results in unstable pooling of fluid above intersections. The release of fluid from the pools was seen to be sensitive to both intersection geometry and steady flow rate. A manuscript documenting these results has been submitted to *Water Resources Research* [Wood et al., 2004b].

9) Collaborated with investigators at the INEEL (J.M. Hubbell, J.B. Sisson, D.L. McElroy) to evaluate the potential for estimating liquid flux at depth in a thick vadose zone consisting of fractured basalt. Shallow estimates of flux are limited by the high degree of spatial and temporal variability present in the near-surface environment. Data from deep tensiometers situated in laterally extensive sedimentary units below and around the Subsurface Disposal Area at the INEEL suggested a much more stable monitoring environment. This approach was found to be limited by a high degree of uncertainty in the estimation unsaturated hydraulic properties from deep core samples. A manuscript co-authored by Nicholl was published in *Vadose Zone Journal* [Hubbell et al., 2004b].

10) R.J. Glass gave an invited talk at the Dedication of the Center for Experimental Study of Subsurface Environmental Processes (CESEP) at the Colorado School of Mines (9/16/2003) on "Process Driven Structure in Subsurface Flow and Transport". His presentation focused on the area of two-phase flow through fractured rock and highlighted important results of slender pathway formation at the network scale and its modeling with Modified Invasion Percolation (MIP) and other approaches.

11) Slender transport pathways have been found in laboratory and field experiments within unsaturated fractured rock. We considered the simulation of such structures with a Modified form of Invasion Percolation (MIP). Results show that slender pathways form

in fracture networks for a wide range of expected conditions, can be maintained when subsequent matrix imbibition is imposed, and may arise even in the context of primarily matrix flow due to the action of fractures as barriers to inter-matrix block transport. Results were published in *Geophysical Research Letters* [Glass et al., 2004].

12) Collaborated with R.M. Holt at the University of Mississippi to develop a special section of the *Vadose Zone Journal* dedicated to the topic of uncertainty in vadose zone flow and transport prediction. The special section includes eight refereed articles and an introduction to the topic co-authored by Nicholl [Holt and Nicholl, 2004].

13) M.J. Nicholl spent July-December, 2003 at Sandia National Laboratories collaborating directly with R.J. Glass on network scale simulations, and supervising experimental efforts to understand behavior in single intersections. In that time we developed procedures for fabricating individual intersections from 3/4" plate glass, and experimental protocols for two phase flow (water into air and TCE into water).

13) To expand our collaboration with the research group led by Dr. Kang-Kun Lee at Seoul National University, the University of Idaho sponsored an extended visit to Sandia National Laboratories by Mr. Sung-Hoon Ji, a Ph.D. student advised by Dr. Lee. Mr. Ji has been an active participant in our laboratory investigation of two-phase flow at individual intersections. Those experiments have uncovered fundamental differences between the invasion of water into an air filled intersection and the invasion of a DNAPL into the same intersection under water filled conditions. For a simple intersection between vertical and horizontal fractures, the intersection acted as a capillary barrier to unsaturated flow. Water accumulated above the barrier, then filled the horizontal fractures before continuing downwards in pulses defined by the barrier. Conversely, the TCE did not invade either horizontal fracture, but instead pooled across the intersection to form a capillary bridge that facilitated downwards migration. Results were presented at a recent meeting of the American Geophysical Union [Ji et al., 2003b], and have been developed into a manuscript that has been submitted to *Geophysical Research Letters* [Ji et al., 2004].

14) Based on the work described in point 13 (above), we designed additional intersection geometries to further explore the substantial differences in behavior between wetting (water into air) and nonwetting (TCE into water) invasion. With continued participation by Mr. Ji, we conducted those experiments at Sandia National Laboratories in the Spring of 2004 and are currently reducing the data.

15) Mr. Benjamin Andre, a Doctoral student from the University of Colorado started working on this research project in Summer 2003. He has developed computer codes for generation and visualization of fracture networks. He spent 2 weeks in October-November 2003 at Sandia National Laboratories, to become familiar with the MIP code for simulation of invasion processes in two-phase flow systems. He is currently working on extending the MIP code to allow for invasion simulations in fracture networks with arbitrarily oriented fractures. Other functionality that is being built in, to the code

includes constraining fractures with other fractures only via intersections, which is critical in the context of the pixelated representations of fractured rock in MIP.

16) Mr. Toshihiro Sakaki, a Doctoral student at the University of Colorado has developed a computational model for simulating the drying of fractured rock masses adjacent to ventilated drifts, in response to air flow through fractures. The modeling approach is based on fundamentally rigorous concepts, especially in regard to mass transfer at the fracture-matrix interface. Preliminary simulations on fracture networks demonstrate the influence of both aperture variability and network topology in generating complex drying patterns and rates.

Planned Activities:

The following tasks are planned for FY05:

1) Mr. Benjamin Andre's effort on fracture networks will be continued to generate three-dimensional networks, and populate individual fractures within the network with variable apertures. The two and three-dimensional generated networks will become the focus for simulations of two-phase flow using the MIP model. During the later part of 2004, Mr. Andre will further develop his thesis research to develop measures of phase structure and phase-diagrams of system behavior in infiltration as a function of fracture network topology and fracture properties.

2) Mr. Sakaki will continue his efforts on simulating drying in fractured rock, and attempt to develop general scaling laws for drying rates in relation to fracture network topology.

3) Complete our evaluation of data from the single intersection experiments, prepare a manuscript documenting the results, and abstract the results for use in the MIP simulations.

4) Complete the development of a mesoscale surrogate fracture network with 171 fracture intersections, perform flow experiments, and prepare a manuscript documenting the results. This work is hoped to demonstrate phenomena characteristic of a Self-Organized Critical System in multi-phase fractured rock environment. An important aspect of this work will be correlating laboratory results to field observations at the INEEL Vadose Zone Research Park.

5) Prepare a manuscript documenting the influence/effect of multiple fracture intersections acting in a single vertical fracture under the conditions of unsaturated flow.

Information Access:

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