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FIELD RESEARCH PROGRAM FOR UNSATURATED FLOW AND TRANSPORT EXPERIMENTATION*

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ABSTRACT

As part of the Yucca Mountain Site Characterization Project, a field research program has been developed to refine and validate models for flow and transport through unsaturated fractured rock. Validation of these models within the range of their application for performance assessment requires a more sophisticated understanding of the processes that govern flow and transport within fractured porous media than currently exists. In particular, our research is prioritized according to understanding and modeling processes that, if not accurately incorporated into performance assessment models, would adversely impact the project's ability to evaluate repository performance. For this reason, we have oriented our field program toward enhancing our understanding of scaling processes as they relate to effective media property modeling, as well as to the conceptual modeling of complex flow and transport phenomena.

I. INTRODUCTION

A key concern facing performance assessment relative to Yucca Mountain, potentially the nation's first high-level radioactive waste repository, is the validity of current models for fluid flow and transport through unsaturated fractured rock. Validation involves the building of confidence in a model's ability to accurately describe a complex physical process in terms of a specified range of boundary conditions and input parameters. Such confidence may not be achieved by simply matching numerical simulation with field and laboratory experimentation. Rather, validation studies should question whether the proper physical processes, in light of key system parameters, have been incorporated into our models. To accomplish model validation according

to this basis requires a more sophisticated understanding of the processes that govern flow and transport within fractured porous media than currently exists.

To address concerns relative to model validation, a research program has been developed for the Yucca Mountain Site Characterization Project at Sandia National Laboratories to investigate mechanisms and processes that govern flow and transport through unsaturated, fractured rock. The research program integrates fundamental physical experimentation with conceptual model formulation and mathematical modeling. Our approach follows five basic steps:

- identify processes governing water flow and radionuclide transport through fractured porous media;
- develop basic scientific understanding of these processes through fundamental conceptual and mathematical modeling, controlled experimentation, and model validation (invalidation) exercises at both the laboratory and field scales;
- 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;
- provide informational needs for site characterization so that the probability of occurrence for each process can be assessed and appropriate model parameters measured; and
- integrate models for important (high probability of occurrence) water flow and radionuclide transport processes into performance assessment codes.

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There are two key elements associated with the model validation program that warrant discussion at this time. First, we approach model validation through an integrated program involving both field and laboratory

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experimentation; our laboratory program also addresses understanding of key flow and transport processes.^{1,2} Secondly, physical experimentation is conducted in both tuffaceous systems associated with Yucca Mountain and in analogue systems where necessary. Because the field program must address a wide variety of physical processes occurring in a variety of rock types (e.g., bedded to densely welded tuffs which vary in their degree of fracturing), there are many situations in which analogue field sites would better suit the experimental program. For instance analogue field sites will be utilized when studying mechanisms responsible for the occurrence of localized saturated zones within otherwise unsaturated media, and in cases where extensive outcrop exposures are not available or accessible at Yucca Mountain (prior to the construction of underground test facilities).

The field research program is prioritized according to understanding and modeling processes, which, if not accurately incorporated into performance assessment models, would adversely impact the project's ability to evaluate repository performance. To meet these ends, two basic objectives have been identified:

- to integrate processes governing rock property variability and scaling into meaningful effective media property models, and
- to develop conceptual models for predicting the occurrence and behavior of localized saturated zones within otherwise unsaturated media.

As described in the next section, strategies for accomplishing the first objective include the sampling of accessible outcrops and the performance of in situ testing to define effective media properties and scaling laws, which will be compared through analysis of the largest-scale experiment. In the subsequent section, we discuss our approach to the second objective, which involves a study of seeps and weeps that represent natural analogues to localized saturated zones that may occur deep within Yucca Mountain.

II. PROPERTY SCALING

Physical properties associated with geologic materials are rarely homogeneous. The spatial variability of properties inherent in a rock mass directly influences the rates of groundwater flow and contaminant transport through natural geologic systems. Variability also gives rise to scale effects related to flow and transport. In mathematical terms, scale effects have been recognized for some time and hence the concept of the Representative Elementary Volume (REV) was developed.³ If the scale of application is different than the scale of measurement, one must make use of intermediate conceptual models, or

scaling laws, that integrate the detailed property spatial variability into effective media property estimates.^{4,5}

We are integrating two approaches to better understand the processes governing rock property variability and scaling in tuffaceous deposits and to incorporate this understanding into credible effective media property models. The first approach involves traditional small-scale outcrop sampling and applies classical statistical and geostatistical methods to define spatial rock-property structure. The second approach, superimposed on the first, measures hydraulic properties for volumes of tuff ranging from sub-cubic meter to tens of cubic meters. Both approaches will define effective properties and scaling laws, which will be compared through analysis of the largest-scale experiments.

A. Outcrop Small-Scale Core Sampling Studies

Three sampling patterns are being used to collect samples in rock outcrop in the primary lithostratigraphic units comprising the unsaturated zone at Yucca Mountain.

1. 1-D Profiles - A very simple approach to understanding spatial continuity is through the collection of samples along one-dimensional profiles.⁶ Such profiles are best collected along the axes of anisotropy as inferred from the geological setting.
2. 2-D Grids - A more comprehensive understanding of spatial variability may be obtained through sampling on a two-dimensional grid. Depending upon the exposures available and the particular goal of sampling, a grid might be oriented in the plane of depositional "bedding" (to investigate lateral continuity and anisotropy) or perpendicular to that plane (to investigate stratigraphic anisotropy).
3. Mixed Patterns - 1-D profiles or 2-D grids can be extended to quasi-2-D or -3-D, respectively, by combining sets of grids or profiles. Such combinations will help utilize the maximum extent of the outcrop in obtaining information relative to the distribution of rock properties. Profiles or grids oriented in the vertical plane will be limited to vertical outcrops such as are found in heavily eroded arroyos or along fault scarps.

Collection of rock matrix samples at the outcrop is performed by coring with a portable core drill. Samples for testing measure approximately 2.5 cm in diameter and 2 to 5 cm in

length. Each collected sample is subjected to a number of analyses. A tentative, and nonexclusive, list of rock properties include the following:

- porosity
- bulk density
- air permeability
- moisture characteristics
- saturated permeability
- relative permeability
- sorptivity

The rock property data obtained from samples of tuff are described using both classical and geostatistical techniques.^{7,8} Specific approaches depend upon the available data and their configuration. In addition to description of correlation lengths, anisotropy, and overall variability, a further objective is to develop material property models for future use in numerical flow and transport codes.

The outcrop sampling activity thus far has provided some 550 samples representing the major rock units composing the unsaturated zone at Yucca Mountain.⁹ Closely spaced (1 to 3 m) samples along vertical transects are supplemented by more widely spaced (30 to 60 m) sampling along stratigraphically horizontal traverses in selected horizons. Preliminary indications are that bulk hydrologic properties are correlated with microstratigraphic subdivisions¹⁰ of the major lithostratigraphic units.¹¹ This correlation is reflected both in a gross change in the mean property within different micro units, and in the range of variograms obtained through quantitative geostatistical evaluation of the vertical transect data. An intriguing, but incompletely explored observation has been the apparently excellent ($r^2 = 0.8$) correlation of saturated log permeability with porosity in tuffs across a wide degree of welding.¹²

B. Variable Scale Experiments

To challenge our understanding of property variability and scaling as characterized in the outcrop sampling studies, we are conducting a variety of tests that interrogate a spectrum of scales in outcrop material. Three types of studies are currently being designed and tested. These include gas-permeameter studies, outcrop corehole studies, and surface infiltration studies.

Gas Permeameter Studies: The gas permeameter studies are designed to interrogate rock volumes from 4 to 7000 cm³, at the outcrop or blocks pulled from the outcrop and slabbed. The technique is rapid, nondestructive, and has been demonstrated in a number of laboratory and outcrop permeability characterization studies at a single scale.^{13,14}

The permeameter consists of a series of valved flow meters and a pressure gauge connected to a source of nitrogen. A sequence of specially designed nozzles, the diameter of which defines

the scale of measurement, is used to establish a known boundary condition on the rock surface. Based on information concerning nozzle geometry, flow rate, and application pressure, the air permeability may be estimated by means of a modified form of Darcy's Law.¹⁵

Initial studies using the gas permeameter are currently being conducted in a controlled laboratory environment. These studies are aimed at defining instrument precision, evaluating the appropriateness of the modified Darcy's Law for computing air permeability, and identifying trends in rock property variability as a function of scale. Data are collected from slabs of densely to moderately welded volcanic tuff (measuring approximately 90 cm by 90 cm by 2.5 cm) that were cut in such a manner as to maximize expression of the anisotropy of the rock. Measurements are taken at four different scales corresponding to inner nozzle-tip-seal radii of 0.63 cm, 1.27 cm, 2.54 cm, and 5.08 cm. These measurements will identify variations in the distribution and correlation structure of the air permeability data as a function of scale. These data also will provide the basis for the formulation of scaling laws to be used in the calculation of effective media properties.

Corehole Studies: Corehole infiltration tests are being designed to be conducted at the outcrop in the coreholes left from the small-scale outcrop sampling studies. These studies will be conducted in the original coreholes as well as in a series of overcored holes, to allow performance of the infiltration studies at a variety of scales. The objective of the tests is to measure hydraulic properties in the larger volume of rock surrounding each hole. First, the gas permeameter will be used to measure permeability. Second, constant-head infiltration tests will be conducted and volumetric flow into the rock measured in time. Using the measured in situ rock permeability, porosity and air entry values measured in the laboratory on the core, and the Mualem mapping¹⁶ between moisture characteristic and relative permeability, the inverse problem will be solved to calculate the relative permeability from the inflow data.

Surface Infiltration Studies: Field infiltration tests will be conducted at scales varying in size from 0.1 to 5 m². Performance of the infiltration tests will involve supplying water at a constant rate by means of an irrigation spray nozzle or at a constant head (ponded infiltration) to horizontal plots or boulders extracted from the outcrop. Tests are expected to last less than two days, during which flow rate will be monitored continuously. A conservative dye will be added to the water to provide information concerning the character of the flow field which develops as a result of the test. Once infiltration has stopped, the site will be carefully excavated. The spatial structure of the dye field will be recorded and

the rock will be intensively sampled to obtain dye concentrations, hydraulic properties, and mineralogical characteristics.

Based on the information gathered during the infiltration tests and application of inverse techniques, bulk hydraulic properties for the rock-mass tested will be established. Such property data will be collected for a variety of rock mass volumes and will be supplemented by laboratory data for sub-cubic meter volumes. Based on the acquired data, efforts will be made to fit scaling models to describe the variability in the bulk parameter values over a range of rock-mass volumes.

C. Analysis

Three types of analyses will be used to compare scaling laws developed from small-scale outcrop sampling and the variable-scale experiments. Common to each of the analyses will be the goal of matching model output with the flow and transport fields resulting from the largest-scale infiltration tests. Different to each of these analyses will be the manner in which the input field (i.e., rock property and hydraulic data) is formulated.

The first analysis will attempt to match flow and transport fields using hydraulic data collected from the site following the infiltration study. Basic interpolation and smoothing techniques will be employed in developing material property models for input into the code. Information gained as a result of this exercise will help evaluate simple interpolation and smoothing techniques and help determine whether the site can be modeled in any detail.

The second exercise will involve the development of effective media property models using classical and geostatistical methods. The effective media property estimates will again be based on data collected from the test site. Efforts will be made to develop property models at scales similar to that of the core samples collected from outcrops and at the scale of the infiltration test site. These exercises will provide a means of evaluating the utility of classical and geostatistical methods to predict spatial variability at scales similar to that sampled and at larger scales.

The third phase of analysis will involve the evaluation of scaling laws formulated from data obtained from the variable-scale experiments. Efforts will be made to use the scaling laws to estimate effective media properties at the scale of the largest-infiltration test based on small-scale measurements made at the test site. These scaling laws are envisioned as providing an alternative or supplemental method for defining effective media properties to that of the traditional or the geostatistical techniques.

III. PROCESS SCALING

Application of the continuum modeling approach and subsequent numerical solution requires choice of the scale at which the problem is discretized and hence the volume over which flow and transport processes are averaged. It follows that as the scale is varied, the relative importance of those discrete processes governing flow and transport may change. Large scale confluence mechanisms are an example.

Current conceptual models of unsaturated flow within fractured rock suggest that under most situations, flow is dominated by the low matrix potentials within the partially saturated rock matrix. High potential gradients pull any water that enters a fracture into the matrix, ensuring minimal fracture flow. Dry fractures form capillary barriers and impede block-to-block flow. If fracture flow occurs, it does so episodically near the surface in response to intense rainfall events where the holding capacity of the surface is exceeded, but dies out rapidly with depth as water is drawn into the matrix. Deep within the formation, localized "perched" saturated zones may occur, as a result of a combination of hydraulic properties, geometry, and flow rates. Fracture flow instigated in the "perched" zones would dissipate with distance as the fracture passes out of these zones and water is absorbed into the matrix.

Contrary to the projections from our conceptual models, persistent saturated conduits for flow within unsaturated fractured tuff formations (seeps and weeps) are known to occur, as exemplified by the presence of seeps in road cuts and weeps in mining drifts associated with otherwise unsaturated country rock. The large scale process of seep and weep formation and possible persistence as a function of system parameters (primarily hydraulic properties of both fractures and matrix, as well as system geometry) and boundary conditions (primarily long-term recharge rates) must be understood.

A natural analogue study of seeps and weeps that occur in the vicinity of the Nevada Test Site (NTS) and at other locations in the western United States is planned. The primary goal of this investigation is to evaluate the feasibility of formulating conceptual models for predicting the formation of zones of localized saturation in terms of relevant system parameters. Although there are no natural springs on the Yucca Mountain Site, this does not lessen the need for addressing their occurrence. In fact, as site investigations move underground, it is possible that weeps will be encountered. Even if this is not the case, these features should be addressed in light of their possible occurrence given changing climatic conditions. To investigate these features, analogue field sites must be identified. Locations with similar geology and similar to slightly wetter climatic conditions

are of primary interest. For example, Cane Spring and Whiterock Spring, located on the NTS,¹⁷ weeps in tunnels in Rainier Mesa (also at NTS),¹⁸ and weeps occurring in mining tunnels near Superior, Arizona¹⁹ all have been identified as possible analogue test sites.

Our approach will be to identify trends which may exist between the occurrence of these features and key system parameters (recharge rate, system geometry, hydraulic properties). This effort will be initiated with a thorough review of the open literature, which is expected to contain much of the information needed. Efforts also will be made to identify seeps and weeps for which published material does not exist, through contact with state highway agencies, mining companies, and other knowledgeable professionals. To augment the acquired information, particular sites then may be selected for instrumentation to collect additional meteorological, hydrological, and geochemical information as deemed necessary. These data will be compiled and efforts made to develop conceptual models to describe the occurrence of the various seeps and weeps as a function of critical system parameters. The conceptual modeling task also will be aided by activities currently under way in the laboratory research program.^{20,21} Such activities focus on understanding the details of the flow and transport processes at the laboratory scale which may be responsible for the occurrence of zones of localized flows in predominately unsaturated media.

IV. CONCLUSION

Potential siting of the nation's first high-level nuclear waste repository is focused on a complex assemblage of fractured and nonfractured volcanic tuffs comprising Yucca Mountain, Nevada. Unsaturated flow and transport through these tuffs is sensitive to both the variability inherent to the geologic material and to the variability in the processes governing flow and transport phenomena. The accuracy of our models is dependent on our ability to define and integrate over the variability in media properties and flow and transport processes. As a result, a basic understanding of the scaling of complex physical processes and heterogeneous site characteristics between the measurement or observation scale and the application scale is felt to be of primary importance to the performance assessment task. In particular, the influence of scaling processes is of concern as they relate to the formulation of effective media models as well as to the conceptualization of complex flow and transport phenomenon such as are responsible for the formation of seeps and weeps. To address this need, a field research program has been developed and described here that is aimed at providing the requisite fundamental understanding and integrating this understanding

into credible scaling models for use in performance assessment.

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