VALIDATION OF REPOSITORY PERFORMANCE ASSESSMENT CODES USING LARGE-SCALE PHYSICAL MODELS

R. Khaleel, J. D. Hoover, T. LeGore, E. C. Thornton,
R. P. Anantatmula, and D. C. Lanigan
Westinghouse Hanford Company, P. O. Box 1970,
Richland, WA 99352

ABSTRACT

Post-closure performance assessment and the associated application of mathematical models play a critical role in assessing the long-term behavior of the engineered and natural barriers of a geologic repository. Although verification and benchmarking constitute an important part of determining model acceptability, it does not establish that the model is a reasonable approximation to physical reality. This is accomplished in the validation step in which model calculations are compared with data from controlled experiments. Although in-situ field experiments provide useful data, information needed for model validation cannot be obtained from field observations alone because of the inherent uncertainties associated with the natural system. However, physical models, when properly scaled, constructed, and instrumented can provide the necessary information for validation of mathematical models and computer codes, and can overcome many of the uncertainties associated with large-scale in-situ testing. The relationships between measurement, size, scaling, and discretization (block size) used in a numerical model must be incorporated in the conceptualization of a physical model. Sizing and scaling requirements of a large-scale physical model for hydrological testing are presented.

INTRODUCTION

The objectives of physical modeling often fall into two categories. The first category is concerned with acquiring a fundamental understanding of the physical processes occurring within a system. The second category is concerned with an evaluation and demonstration of the applicability of the mathematical modeling process to describe the results of physical experiments. Such experiments, often referred to as validation experiments, are particularly useful for confirmation of a site's suitability for long-term isolation of nuclear wastes. A successful validation of model simulations with experimental data indicates that the model is a reasonable description of physical reality and accurately incorporates the interrelationships among the various processes. However, as concluded in a recent HYDROCOIN (Hydrologic Code Intercomparison Study) workshop, the data bases for validation experiments are virtually nonexistent (1):

> "Extensive worldwide literature searches
> and inquiries of experimentalists within
> and outside of HYDROCOIN group indicated that experiments adequate for
> model validation do not exist"

In a cooperative effort, Ishikawajima-Harima Heavy Industries Co., Ltd. (IHI), Japan and the Nuclear Waste Department (NWD) of the Westinghouse Electric Corporation are studying the feasibility of constructing and utilizing large-scale physical models in an above-ground geologic test facility for the purpose of validating repository performance assessment codes. This paper presents sizing and scaling requirements of a large-scale physical model for hydrological testing.

MODELING AND MODEL VALIDATION

There are five steps in a modeling effort related to post-closure performance assessment of a geologic repository: conceptual formulation, mathematical formulation, numerical modeling, verification and benchmarking, and validation. The first step consists of a conceptualization of the physical system. The conceptual model consists of a set of assumptions that translate the physical problem and the real domain to simplified versions that are acceptable in view of the objectives of modeling and the associated physical problem.

In the second step, the conceptual model is expressed in the form of a mathematical model. The latter includes a definition of the geometry of the considered flow domain and its boundaries, applicable mass, momentum and energy equations, equations of state, and boundary and initial conditions.

The third step is the solution of the mathematical model using appropriate analytical or numerical methods. Frequently, because of the irregular shape of the domain's boundaries, the heterogeneity of the domain, and the irregular temporal and spatial distributions of the various excitations, or source-sink functions, numerical methods are employed to solve the mathematical model. Because of the large number of equations that have to be solved simultaneously, a computer code has to be developed in order to obtain a solution.

The next step is the verification that the solution of the numerical model is correct and involves checking for mathematical or programming errors. Numerical solutions are best verified by comparison with available analytical solutions. In the absence of analytical solutions for verification purposes, an intercomparison of several codes, a process called benchmarking, for the same physical problem is performed.

The final step compares the solution of the mathematical model to the physical reality which it claims to describe. Validation, as defined by the International Atomic Energy Agency, is:

"A conceptual model and computer code derived from it are 'validated' when it is confirmed that the conceptual model and the derived computer code provide a good representation of the actual processes occurring in the real system. Validation is thus carried out by comparison of calculations with field observations and experimental measurements."

VALIDATION ISSUES

Model validation can be thought of as a series of questions to be asked of the physical experiments, experimental database and the mathematical models used to simulate various processes (2):

1. What are the relevant processes of the experiment and how does the model consider them?
2. What is the geometric and spatial framework of the hydrogeologic system and do the modeling assumptions conform to them?
3. Are the simplifying assumptions inherent in the model compatible to the hydrogeologic, hydraulic, and geochemical components of the system being modeled and consistent with model use?
4. Are the model inputs representative of the system?
5. Are the field and laboratory experiments detailed enough to provide unique sets of databases that characterize the governing processes?
6. Is the measurement scale compatible to the scale of the relevant processes?
7. Is there a coherent validation strategy that allows for additional data collection and determination of "goodness of fit" criteria for comparison of the simulation results versus the independent experimental database?

For the purpose of validation, laboratory analogs of natural systems must consider a scale large enough to include a "representative sample" of the rock mass. If natural groundwater systems, for example, were truly homogeneous, characterization and validation would be much simpler. A single measurement for parameters would suffice and the scale of the laboratory sample or numerical discretization would not be as important. However, natural groundwater systems are never truly homogeneous. Therefore, a validation experiment for hydrology must consider the heterogeneous nature of natural groundwater systems.

It should be noted that, although in-situ field experiments provide useful data, information needed for model validation cannot be obtained from field observations alone because it is not possible to adequately define the heterogeneities existing in the real system. It is also generally agreed that small and medium scale physical models may not adequately represent the field-scale heterogeneities. However, large-scale physical models, when properly scaled, constructed, and instrumented, can provide the necessary information for validation of mathematical models and computer codes.

Furthermore, it is important to note that the scale of observation dictates whether a phenomenon is to be considered as random or deterministic (3,4). A phenomenon (e.g., a dynamic variable) can be considered random on one scale and deterministic on another. For example, it is common to assume that the "hydraulic conductivity" is random on the field scale yet deterministic on the laboratory scale. From a measurement perspective, in the laboratory, it is easy to control the scale of heterogeneity. To the contrary, in the field, we have no control over heterogeneity and therefore hydraulic conductivity has to be considered random.

The relationships between measurement, size, scaling, and discretization (block size) used in a numerical model must be incorporated in the conceptualization of a physical model. Sizing and scaling requirements of a large-scale physical model for hydrological testing are presented in the following sections.

VARIOUS SCALES IN SUBSURFACE FLOW

Before detailing our approach on sizing of the physical model, it is appropriate to review the various scales that are frequently used in subsurface flow, and their relation to hydrologic measurements. The following discussion on scales is essentially based on (5).

Subsurface flow domains are characterized by a length scale of their spatial extent and three such scales are of fundamental importance in flow through porous media: a. the laboratory scale; b. the local scale, and c. the regional scale (5). The laboratory scale, characterizing the dimensions of common experimental setups, is of the order of 0.1 to 1 meter. Figure 1, the experimental set-up used by Darcy to investigate the flow of water in vertical homogeneous sand filters, is an illustration of the laboratory scale.

In porous media, flow occurs through a complex network of interconnected pores, or openings. However, when dealing with flow in porous media, we overlook the microscopic flow patterns inside individual pores and consider some fictitious average flow which takes place in the porous medium comprising the aquifer. By doing so, we employ the concept of a continuum. The obvious reason for employing the continuum approach in flow through a porous medium is that it is practically impossible to describe in any exact mathematical manner the complicated solid surfaces that bound the flowing fluid (6). At the scale of the Darcy experiment (Fig. 1), the medium is regarded as having the behavior of a homogeneous medium. The continuum approach as implied in a Darcy experiment is commonly illustrated with a diagram such as Fig. 2. The volume at which the parameter of interest (porosity in case of Fig. 2) ceases to vary is defined as the representative elementary volume (REV). With respect to porosity, the REV of a medium can be sought by measuring the porosity of increasing volumes of rock until the value does not change significantly with the addition or subtraction of a small volume of rock.

The local scale is much larger than the laboratory scale and is of the order of aquifer thickness (i.e., 1 to 100 meters) in the vertical direction and of the same order in the horizontal plane. Generally, at this scale the flow or the transport processes are of a three-dimensional nature. Figure 3 is an illustration of a local, inhomogeneous, layered aquifer with a gradual variation of hydraulic conductivity in the vertical (z) direction.

The regional scale, of the order of 10^3 to 10^5 meters in the horizontal plane, is much larger than the aquifer thickness and the flow variables are averaged over depth, such that flow is two-dimensional in the plane. Figure 4 is an

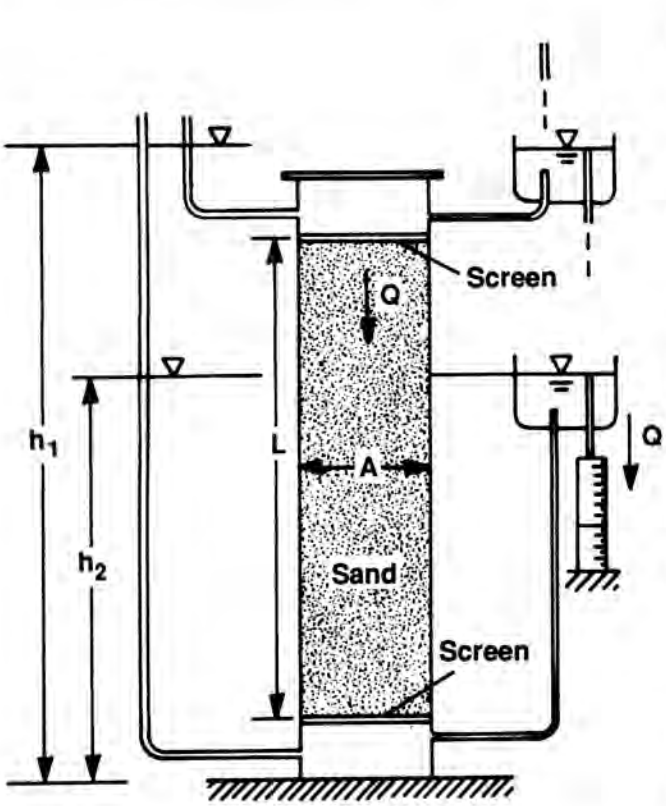

Fig. 1. A Laboratory Scale (Macroscopic) Model.

example of a regional aquifer system with multiple aquifers and aquitards.

In physical problems, the variables of interest are defined by a process of space averaging over a volume surrounding a point with coordinate x. In case of local scale, the point values are defined by averaging the variables over a volume containing many pores, a volume which is extremely small compared to the local domain size. Therefore, the macroscopic (REV-averaged) variables measured at the laboratory scale become now "point values" and we can ignore the pore-scale heterogeneity (5). In physical terms, the fluid flow obeys, for instance, Darcy's law and the hydraulic conductivity K is a function of x, K being defined on a laboratory sample surrounding x.

At the regional scale, point values are defined by a space average over a volume of the order of the local scale, i.e., the depth of the aquifer. The flow equations are now defined in terms of transmissivity T, and T(x) is the value of T determined by a well test at x. At regional scale, we can ignore the local scale heterogeneity.

SIZE OF PHYSICAL MODEL

The justification for the minimum size of a physical model for hydrological testing can be based on the nature of heterogeneities introduced into the model. Numerical simulations are utilized to determine the size of the model. The following procedure is specifically used for porous medium models.

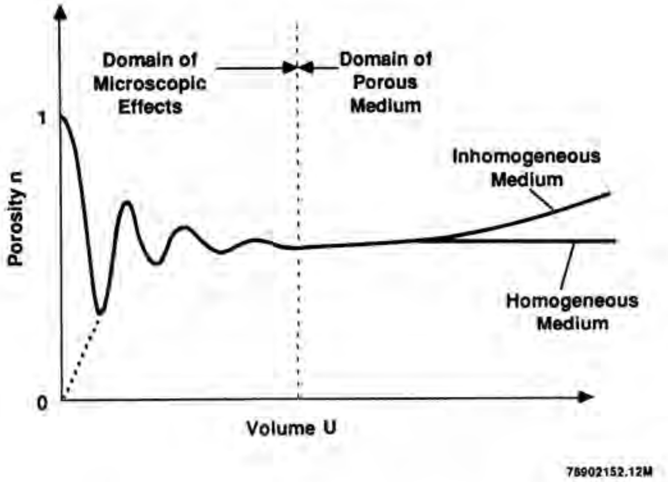

Fig. 2. Definition of Porosity and Representative Elementary Volume (REV).

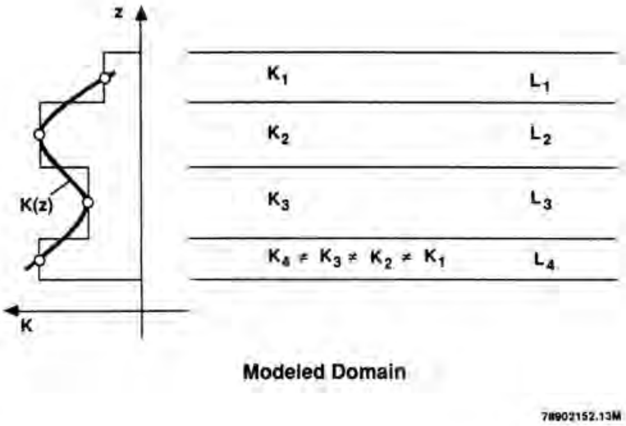

Fig. 3. A Local Aquifer System.

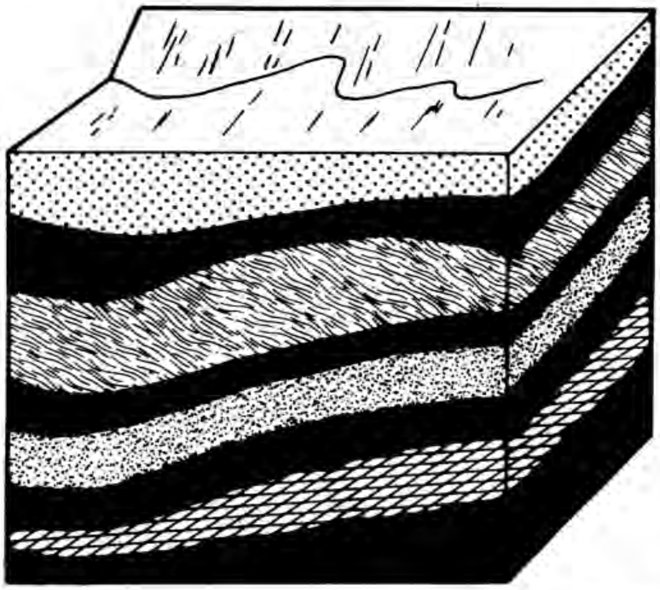

Fig. 4. A Regional Aquifer System with Multiple Aquifers and Aquitards.

After a model geometry has been generated (generation region) and hydraulic conductivity values have been assigned randomly to various blocks using a lognormal distribution with a prescribed mean and variance, a number of flow regions are selected within the generation region. A flow region is a window within the larger geometry. Boundary conditions are assigned to generate a uniform head gradient along the length of each flow region. A groundwater flow code is used to compute the steady-state head distribution within each flow region.

The following two criteria are used to analyze the numerically computed head distribution data obtained for various flow regions. The first criterion considers the variance of head distribution at several sections within the model. As the scale of the model is increased, for the same prescribed hydraulic conductivity distribution, the variance of head distribution should approach a relatively constant value.

The second criterion evaluates the computed equivalent hydraulic conductivity values for various flow regions. As the scale of the model is increased with each flow region, the equivalent hydraulic conductivity, based on computed head distribution, should approach a relatively constant value. In other words, the sample introduced into the physical model should be large enough to contain a representative sample of media heterogeneities. The flow region that satisfies the above two criteria yields the desired length of the hydrology model.

SCALING RELATIONSHIPS

The hydrology physical model is a scaled-down model of the prototype aquifer. Relationships are determined between two groups of variables and coefficients, in order to predict the behavior of the prototype from experiments performed on a model that represents it. In other words, heterogeneity due to permeability or porosity variations in the prototype are simulated by varying the corresponding properties of the material used in the model according to scaling rules (6).

The experimental results from physical model are presented in terms of dimensionless parameters. The relationships among the model and prototype scales can be used to derive the dimensionless parameters. When the experimental results are expressed in terms of the dimensionless parameters, the resulting relationships can be extended to a wide range of cases of the same phenomenon, but with different values of the parameters involved. Therefore, although a specific set of experiments will be conducted in the physical model, the experimental results and the use of scaling laws will provide an important extension to other conditions not analyzed in the laboratory.

CONCLUDING REMARKS

Laboratory analogs of natural systems must be able to simulate the hydrogeochemical processes occurring in a natural system as closely as possible. Laboratory bench-scale tests often do not provide accurate analogs of natural systems. Large-scale physical models can provide a more accurate representation of the processes that are expected to occur in the near- and far-field repository environment.

Although the focus of this work has primarily been on the hydrology physical model, appropriately scaled models are also needed for model validation in areas such as geochemistry, geomechanics, and corrosion.

Geochemistry. Many existing laboratory experiments conducted to evaluate rock-water interaction in flow-through systems have not been properly designed with respect to minimum column residence time. This drawback may be alleviated by considering the kinetics of the geochemical processes and the minimum achievable flow rates, and by evaluating minimum size and time requirements (7).

Geomechanics. A knowledge of rock mass properties and thermomechanical response is required as input to mathematical models used to predict the time dependent behavior of the near-field host rock surrounding the excavated openings in a geologic repository. The deformational behavior of rock materials is, however, dependent upon the scale of volume of rock being investigated. The behavior of small, intact specimens of rock is likely to differ significantly from that of large specimens with many discontinuities. Therefore, geomechanics experiments should consider the material behavior on a scale large enough to representative sample limitations associated with small-scale laboratory testing in geomechanics.

Corrosion. Laboratory test data on container corrosion are frequently obtained from small specimens where temperatures are fairly uniform. However, in a larger scale container, temperature gradients existing across the surface can have significant effects on corrosion mechanism. Therefore, it is important to validate corrosion performance assessment codes using large-scale physical models (e.g., half the size of the prototype) in order to accurately predict the long-term corrosion behavior of the container exposed under repository conditions.

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