THE ROLE OF LARGE-SCALE TESTING IN PERFORMANCE ASSESSMENT OF A HIGH LEVEL WASTE REPOSITORY

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ABSTRACT

Properly scaled and sized tests are required in assessing the long-term performance of a nuclear waste repository. The processes expected to occur in the repository and computer codes used to predict behavior and conditions are evaluated using laboratory and field tests. An accurate representation or simulation of processes in a test environment often require the physical size of the test to be relatively large. The size of existing and proposed tests, therefore, requires evaluation of their ability to provide representative results.

A methodology for evaluation of the adequacy of test size is proposed that is similar to the performance assessment process itself. This methodology has been applied to scaling requirements for geochemistry and hydrology physical models. The approach for determining the minimum size requirements for a flow-through test apparatus is presented as an illustrative example of this procedure. Such an approach can be used to evaluate the size requirements in most categories of testing. Tests conducted without evaluation of the sizing and scaling requirements can yield unrepresentative or erroneous results that may compromise assessment of repository performance.

INTRODUCTION

The performance assessment process is a structured process used to evaluate the performance of a nuclear waste repository. Assessment of the radionuclide isolation capability of a repository is one objective of the process. This process is also intended to guide site characterization and associated field and laboratory testing. The roles of testing in the performance assessment process are illustrated in Fig. 1. These roles include: 1) refinement and validation of process conceptual models for repository phenomena; 2) characterization of process functional relationships; 3) generation of data unobtainable by other methods; 4) validation of computer codes.

The first objective of this paper is to identify the importance of evaluating the adequacy of repository tests with respect to their size and scale. The second objective is to present an approach for the evaluation of appropriate test size, and to provide an example of its application. The capability of a test to provide results that are representative of the processes of interest, is not commonly evaluated, but such evaluations have important ramifications to the performance assessment process and particularly to code validation. The representativeness of a test often relates to its physical size and scale. In many cases, representative tests are required to be relatively large, and are referred to as large-scale tests. Because the cost, time, and facility requirements of large tests can be prohibitive, a determination of the minimum size requirements for representative tests should be considered an important part of a testing program.

A general approach for evaluating the size of an experiment is presented in this report. The application of this methodology to the size analysis of a flow-through hydrothermal test apparatus is also examined.

IMPORTANCE OF TEST SCALE

The scaling terminology used in this report is briefly defined for the purpose of clarification. Small-scale tests refer here to the physical size of conventional bench scale apparatus and that are commonly on the order of centimeters. Unscaled tests refer to tests performed with apparatus for which the appropriateness of the scale has not been evaluated. Unscaled tests may be small or large. Large-scale refers here to tests that are relatively larger than the conventional scale. Large-scale tests may be very large for some types of tests, such as a hydrology tank measuring several hundred cubic meters in volume. However, a moderately sized test column measuring a few meters in length may be regarded as relatively large-scale in comparison to conventional apparatus measuring several tens of centimeters in length.

The general requirement for testing in all disciplines is that the test conditions and parameters provide for an accurate representation or simulation of the processes and phenomenology of interest. This requirement of representativeness is the principle justification for tests of appropriate size.

Conventional small-scale experiments can provide useful insights into the phenomenology of many processes in a manner that requires less time and cost than large-scale tests (1,2), and that do not require development of new technology or techniques. However, the necessity of using representative volumes or physical sizes to adequately represent the conditions or processes of interest are well documented in the areas of hydrology and geomechanics testing (3,4). The same requirement of representativeness for test conditions (e.g., volume, mass, flux, or time related physical parameters), applies to testing in all disciplines, including large-scale field testing or in situ testing, and especially to tests involving coupled processes (i.e., combinations of thermal, hydrologic, chemical, or mechanical processes).

Although the scale of testing in some disciplines has been the subject of considerable discussion, the consequences of unscaled tests have received relatively less attention. Tests have, in many cases, been performed using existing conventional equipment that may or may not be of adequate type or size to provide appropriate data. However, the type and extent of the inadequacies, if any, are generally not known. Tests performed with apparatus that do not

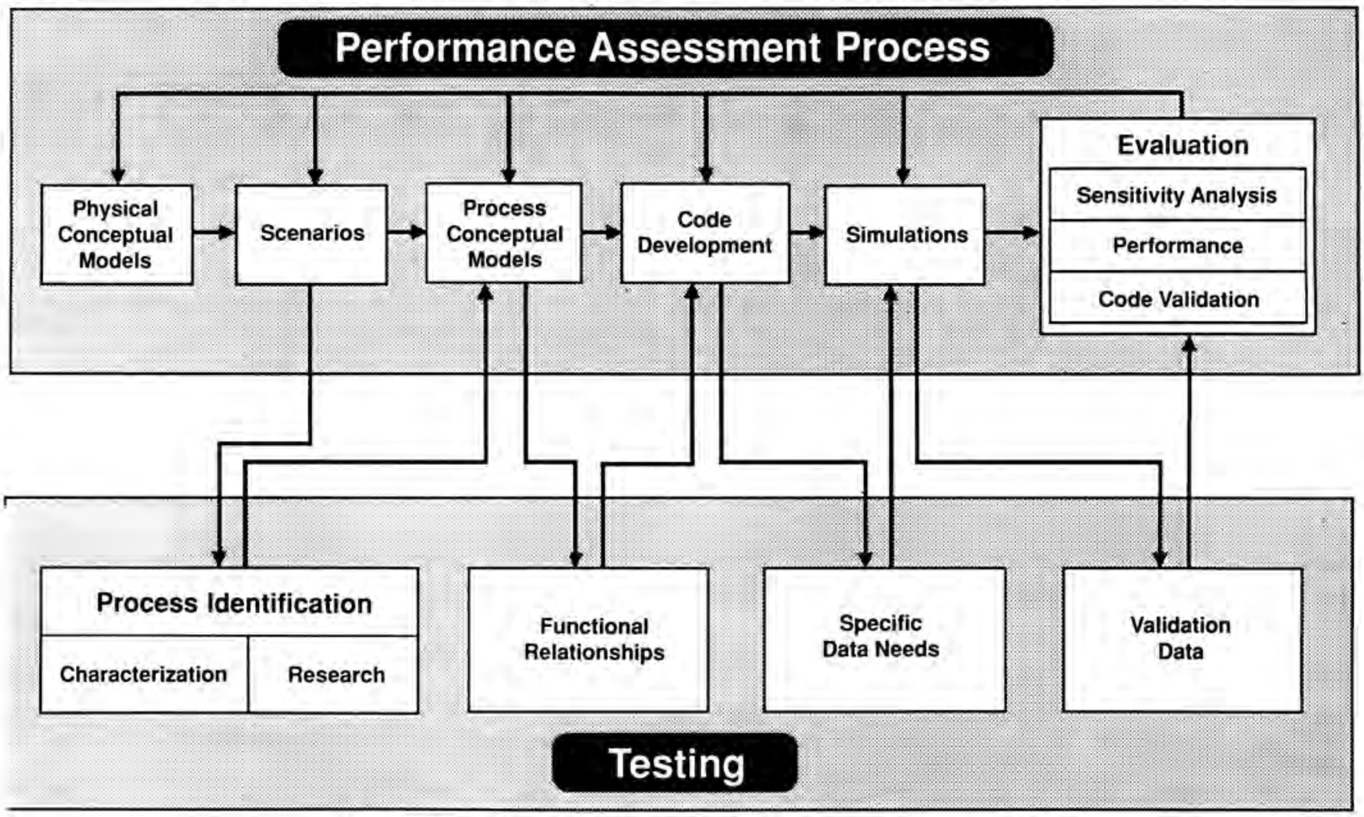

Fig. 1. The Roles of Testing in the Performance Assessment Process.

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adequately represent the processes or conditions under investigation can yield unrepresentative or misleading results that hinder, rather than further, efforts of evaluating repository performance. Unrepresentative test results can also lead to erroneous conclusions regarding the performance of the repository or its subsystems.

It is indicated from the general scaling and sizing requirement of representativeness that all tests should be of appropriate size to achieve their designed purposes. It follows that the adequacy of existing tests requires evaluation, and that similar evaluations should guide the design and construction of new tests. An evaluation of the test size or scale adequacy is, therefore, clearly required. An example of a general approach for this evaluation is proposed in the following section.

GENERAL APPROACH FOR EVALUATING TEST SIZE

A general procedure has been developed in the study of sizing requirements for geochemistry and hydrology tests, that provides a basis for the determination of appropriate minimum test scales. The basic steps in this procedure are similar to those in the performance assessment process itself. These steps include:

- Identification of the conditions and processes to be investigated
- Qualitative assessment of experiment (conceptual models)
- Determination of size limiting parameters
- Assessment of test parameters
- Mathematical description of processes/conditions in terms of apparatus size
- Identification of key sizing terms
- Solution of mathematical model(s) constraining minimum physical size

Identification of the processes and phenomena to be investigated, and the conditions under which they are to be investigated, is fundamental to the evaluation of test scale. This step relates directly to the development of scenarios and process conceptual models in the performance assessment process (Fig. 1). The development of qualitative models or conceptual models for tests assists in the identification of phenomena that should be considered in the scale evaluation, and also aids in assessing the consequences of tests performed at inappropriate scales. In some cases, the required apparatus scale can be roughly constrained, i.e., the adequacy of smaller versus larger scale. This step is also important in the development of functional relationships for the mathematical formulation regarding minimum appropriate scale.

Test parameter identification, and the identification or estimation of mathematical expressions that describe the fundamental relationships of individual processes, are related activities. The fundamental sizing or scaling parameters are identified from these expressions and/or from the conceptual test model. Parameters such as representative volumes in hydrology and geomechanics tests, or residence time in a reaction vessel for geochemistry tests, are examples of key scaling parameters.

An evaluation of assumptions that can be made, and manipulation of mathematical and numerical models to describe processes in terms of common or key sizing parameters are then performed. An example of the application of this process is provided in the following section. An example of the manner in which minimum appropriate size of the test apparatus can be determined is also illustrated.

APPLICATION OF METHODOLOGY TO GEOCHEMISTRY FLOW-THROUGH TESTS

An application of the test scaling methodology for determination of the minimum size requirement of a geochemistry test apparatus is illustrated for a simplified test case. The example provided here utilizes the general methodology outlined above in determining minimum size requirements of flow through a hydrothermal reaction column used in evaluating coupled reaction and transport processes in open hydrothermal systems. The flow-through experimental apparatus is shown conceptually in Fig. 2. The apparatus consists of a cylindrical metallic column containing a porous material, such as rock or minerals, that is subjected to interaction with synthetic groundwater passing through the column under fixed conditions (e.g., temperature, pressure, flow rate, porosity, etc.).

Many processes can be investigated with this type of apparatus. Processes most commonly evaluated by use of flow-through apparatus include: mineral and/or metal dissolution; precipitation of secondary minerals; mineral redistribution; mass transport of dissolved and suspended components; sorption reactions; reaction kinetics; colloidal reaction and transport; and oxidation/reduction reactions. The coupled processes of mineral dissolution and precipitation in an open flow-through system are considered here for the purpose of illustrating the methodology of evaluating test scale.

The parameters necessary for evaluation of minimum appropriate test column size are of two types: 1) parameters involving the dimensions and test conditions associated with the apparatus; and 2) parameters associated with the reaction and/or transport processes of interest. The parameters used in this example are identified in Table I.

The qualitative assessment (i.e., conceptual models) of flow-through *experiments* involves consideration of the consequences of significant variations in flow-rate and residence time. It may seem intuitive that the dominant rate of mass transport should affect the rates of irreversible reactions, and that processes such as open system dissolution, precipitation, and sorption are dependent on such parameters. However, experimental results confirming these relationships have only recently been reported (5). Scenarios based on these relationships suggest experiments with flow rates that are very fast, and/or residence times or column lengths that are short, are applicable to dissolution without precipitation. On the other hand, test conditions involving low flow rates combined with long column lengths require very long residence times (i.e, run times), and are, therefore, impractical. The optimal combination of apparatus dimensions and test conditions required for valid testing, however, requires quantitative evaluation.

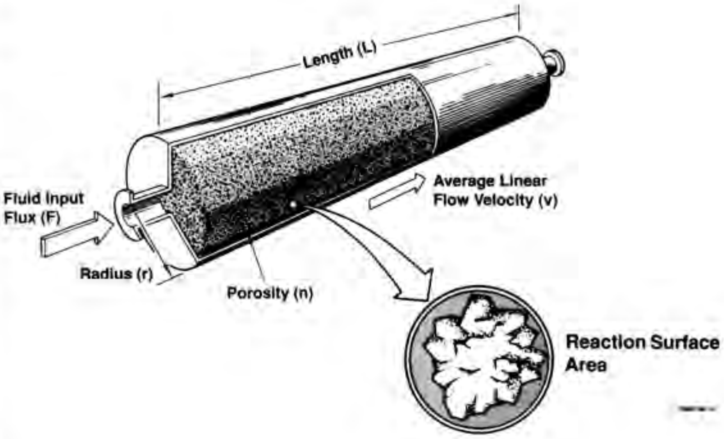

Fig. 2. Schematic Representation of a Flow-Through Column and Apparatus Parameters.

The mathematical descriptions of processes and test conditions under consideration include: an expression relating the average linear flow velocity (v) in the column to the total fluid flux (F), cross sectional area of the test column, and media porosity (n), Eq. (1); an expression relating this flow velocity to column length and residence time, Eq. (2); a transition state theory expression involving mineral dissolution and saturation terms as a function of concentration, time, temperature, and effective surface area, Eq. (3); and an equation describing mass transport, Eq. (4). The various terms in these equations are defined in

$$v = F/npr2 \qquad \text{(Eq. 1)}$$

$$t = L/v = npr2L/F \qquad \text{(Eq. 2)}$$

$$D = dC/dt = K'(A/V) \exp[(-\ln(Keq/Q))/s] \qquad \text{(Eq. 3)}$$

$$dC/dt = D - v\, dC/dx \qquad \text{(Eq. 4)}$$

TABLE I

Flow-Through -Test Parameters

Apparatus and Test Condition Parameters

r = column radius
L = column length
F = fluid flux
n = media porosity
T = temperature
P = pressure
A = reactive surface area
V = fluid volume
t = time (residence time)

Reaction and Transport Terms

K′ = dissolution rate
K_{eq} = equilibrium constant
v = average linear flow velocity
C = concentration
C_{sat} = concentration at saturation
x = distance
Q = activity quotient
s = stoichiometry coefficient

A number of assumptions are commonly made regarding test conditions or test models that can be used in developing mathematical and numerical models for the scaling evaluation. For example, the sizing of the flow-through column includes assumptions regarding the processes involved (e.g., dissolution, precipitation, transport); dynamics of flow (e.g., plug flow); the number and type of participating species (fluid and solids); the nature of the reactions; the test conditions (e.g., temperature and pressure ranges, effective surface areas, flow rates, run times); and engineering limitations (e.g., minimum flow rate and maximum pressure constraints). Other assumptions are also made concerning the manner in which the system is to be modeled. In this simplified example, the stoichiometry term (s) in the transition state expression is set equal to 1.0, precipitation kinetics are ignored, and the model is assumed to represent the dissolution and precipitation of a homogenous solid (e.g., quartz). It is also assumed that in the simplest case, the minimum time required for precipitation in this system would be the same as that in a closed system, i.e., $dC/dt = D$.

In most geochemical tests, the key process for determining size limitations involves the time required for the slowest process or reaction to occur or proceed to steady state. In this model, the precipitation requirements of the secondary mineral(s) of importance (i.e., conditions of saturation) constrains the minimum apparatus size.

A key step in the evaluation is then the expression of the processes/phenomena in terms that can be related to the physical size of the apparatus. In this case, the key relationship is the calculation of residence time because residence time is related to column length, the rates of reaction/dissolution, to the time required for saturation/precipitation, and the change in concentration of species in solution as a function of time (dC/dt). For this simplified case, the time parameter represents the residence time in the column. Equation 5, obtained from the integration of Eq. (4) with respect to time, is an expression that can be used to determine the minimum residence time required for precipitation to occur in the test column.

$$C = \mathrm{Csat}\,(1-\exp[-K'(A/V)]) \qquad \text{(Eq. 5)}$$

Precipitation of a secondary mineral species is a function of the concentration of the species in solution. It is assumed in this case that precipitation results when the fluid is saturated. The time required for saturation, therefore, constrains the minimum residence time and the physical dimensions of the apparatus. A graphical representation of model solutions for these relationships is illustrated in Fig. 3.

A similar approach can also be applied in evaluating the size requirements of more complicated systems. Models such as those presented by Lichtner and others (6) and Lichtner (7) for Lagrangian and Eulerian formulations describing the metasomatic processes associated with open-system mass transport and fluid-rock interaction yield results that can be handled in a similar manner as illustrated in Fig. 3.

SUMMARY

Laboratory testing has many roles in assessing the long term performance of a nuclear waste repository. Tests in both the laboratory and in the field are required to accurately represent the processes and conditions for which the tests are designed. It is therefore implied, that tests of appropriate size and scale are required to meet this representativeness requirement for the tests and test results. Improperly scaled tests or tests that do not adequately represent the processes of interest seriously compromise the performance assessment process.

Existing tests and proposed tests, therefore, require evaluation of the adequacy of their size or scale. One approach to this evaluation is a methodology similar to that of the performance assessment process itself. This general evaluation procedure has been successfully applied to the determination of minimum size requirements of geochemistry test apparatus (flow-through reaction column) and hydrology testing (8). It is indicated from the results of this work that this general methodology can also be applied to the evaluation of test scale in other disciplines such as geomechanics and corrosion testing.

ACKNOWLEDGEMENTS

This work was carried out as part of a joint study between the Ishikawajima-Harima Heavy Industries Co., Ltd. (IHI) and the Nuclear Waste Department of Westinghouse Electric Corporation. Part of this study was performed under the contract between the Power Reactor and Nuclear Fuel Development Corporation (PNC) and IHI.

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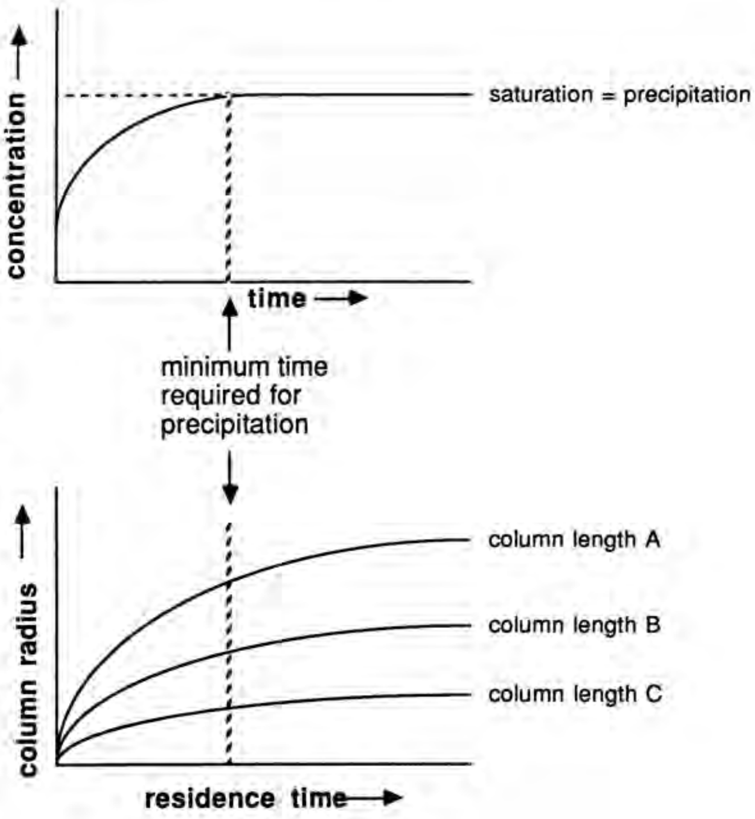

Fig. 3. Schematic Model Solution for Minimum Required Size of a Flow-Through Column.