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Approaches for the Validation of Models Used for Performance Assessment of High-Level Nuclear Waste Repositories

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ABSTRACT

The purpose of this report is to provide general approaches and concepts that can be applied in validation of models used in performance assessment of high-level waste (HLW) repositories. The approaches are based on a validation strategy that Sandia National Laboratories (SNL) has implemented as participants in the International Transport Validation Study (INTRAVAL). This strategy focuses on the demonstration that performance assessment models are *adequate* representations of the real systems they are intended to represent, given the pertinent regulatory requirements rather than proving absolute correctness from the purely scientific point of view. Positions that are taken consist of the following: (1) due to the relevant time and space scales, models that are used to assess the performance of a HLW repository can never be validated; therefore, (2) validation is a process that consists of building confidence in these models and not providing "validated" models; in this context, (3) model validation includes comparisons to "reality," however, adequacy for the given purpose (assessing compliance with regulations) is the overall goal; (4) comparisons to "reality" consist of comparing model predictions against laboratory and field experiments, natural analogues, and site-specific information; (5) when comparing experimental data to model predictions, a model can be either "invalid" or "not invalid," based on the null hypothesis concept, however, confidence in the model arises in finding a model to be "not invalid" over a wide range of conditions; (6) an attempt should be made to consider in the validation process all plausible conceptual models; and (7) when comparing experimental data to model predictions, a logical systematic approach should be followed (i.e., model input tested separately from model structure). This report discusses (1) the definition of validation in the context of performance assessment for HLW repositories, (2) the need for validation, (3) an approach to validation, and (4) an approach to comparing model predictions with experimental data proposed by the authors.

CONTENTS

FOREWORD

This report presents the views of the authors on the validation of models for performance assessment of HLW repositories. The intent of presenting these views is to provide concepts that may be considered by the U.S. Nuclear Regulatory Commission (NRC) in formulating positions on model validation. The views are not necessarily those of the NRC. Therefore, it should not be construed that following the approaches presented in this report will result in acceptance of specific performance-assessment models by the NRC in the licensing process.

1.0 INTRODUCTION

To obtain a license for a high-level radioactive waste (HLW) repository, the Department of Energy (DOE) will carry out a program of site characterization and performance assessment analyses to demonstrate with "reasonable assurance" that burial of HLW wastes will pose no undue risk to the public health and safety. No direct means of assessing the behavior of a repository system exists because of the size of the area of regulatory concern (more than 100 square kilometers) and time scales involved (10,000 to 100,000 years). Therefore, it is expected that the DOE will use a wide variety of mathematical and numerical models, and associated computer codes, to complete the required analyses. Rendering the analyses defensible will require the models and data used for the performance assessments to be sufficiently representative of the repository system, including the engineered barrier and the natural barrier. The DOE is responsible for ensuring the validity of the models and codes used, the quality of data, and the adequacy of the overall analyses.

The U.S. Nuclear Regulatory Commission (NRC), on the other hand, is responsible for evaluating the DOE's license application and deciding whether to grant such a license. Therefore, the NRC must be able to judge whether the DOE has demonstrated that the models are representative of the repository system conditions. Sandia National Laboratories (SNL) has been responsible for developing and examining models that the NRC could use in an independent evaluation of a HLW repository license application. Therefore, the NRC, under the HLW Performance Assessment Technical Assistance Project (FIN A1165), contracted SNL to provide a document discussing model validation. This report provides NRC with a philosophy on model validation and the validation process.

2.0 DEFINITION OF VALIDATION

There are several definitions for the term "validation." NRC [1984] defined validation as the process of obtaining "assurance that a model, as embodied in a computer code, is a correct representation of the process or system for which it is intended." DOE [1986] defines validation as "a process whose objective is to ascertain that the code or model indeed reflects the behavior of the real world." Others (e.g., Borgorinski and others, 1988) follow the International Atomic Energy Agency's definition that validation is confirmed when the model and computer code "provide a good representation of the actual processes occurring in the real system." In this report, NRC's definition of validation is used, however, all the definitions of validation are consistent, although derived from different perspectives. That is, they all are concerned with providing assurance that a model represents reality. This is different from the classical scientific approach which consists of proposing a hypothesis and then designing tests to disprove that hypothesis. Thus, science is not concerned with validating models but, rather, invalidating them. The premise in this report is that one can never prove that a HLW performance assessment model is "valid"; therefore, a model can only be declared "invalid" or "not invalid." More than 30 years ago Popper [1958] perceived that "...whenever we propose a solution to a problem, we ought to try as hard as we can to overthrow our solution, rather than defend it." This idea also has a basis in ordinary statistics whereby one proposes an idea, then attempts to disprove it by testing the null hypothesis. This philosophy has a counterpart in the U.S. judicial process where the null hypothesis is that one is "not guilty." A jury must either fail to reject the null hypothesis (the individual is "not guilty"), or reject the null hypothesis (not "not guilty"). Clearly, just because an individual is judged not guilty does not mean that the person is innocent. It simply means that there was enough evidence for the jury to fail, beyond a reasonable doubt, to reject the null hypothesis. In model validation, this is analogous to the model being "invalid" or "not invalid." Hence, from a regulatory perspective, declaring a model "not invalid" does not guarantee validity. It only provides a means for the modeler to demonstrate that the model is not incorrect. Showing that a model is not incorrect builds confidence in the model and acknowledges that perfection (i.e., validated performance assessment models) is not possible.

The desire for validated models arises from a decision-making framework, either for designing a repository or for providing assurance that the assessment of long-term repository performance is meaningful. In licensing a HLW repository, the distinction between a scientific approach to developing and testing models and the regulatory approach for validating models is critical. For one, the pure scientific approach, generally, would ask for a complete and detailed explanation for all observed phenomena and is not concerned with the specific application of science. Whereas, the regulatory approach would ask only for an adequate description of the phenomena for a given purpose (e.g., for the licensing of a repository). Thus, a bounding or conservative model may be adequate for regulatory purposes but, by definition, not provide a detailed description of all phenomena. This is not to say that the scientific process is not followed in the validation of models used in the regulatory arena. The scientific process is a subset of the regulatory validation process. However, since the scientific process is not necessarily tied to an application, the final decision as to the adequacy of a model will be based on regulatory, not scientific considerations. The scientific process does not have to go as far as determining the adequacy of models for a specific purpose, whereas the regulatory process must.

Models that are used in a performance assessment are a combination of the site-specific data that describe a particular geologic setting or experiment, and the physical process models contained in the relevant computer codes. Hence, the term model, as defined herein, includes the conceptual model, the mathematical model, the computer code and its associated input data. Therefore, validation of performance assessment models is ultimately a site-specific issue. However, the testing of models of various geologic media will aid in gaining (or losing) confidence that the process models contained in the codes are adequate representations of what is occurring in nature.

The goal of a model-validation exercise should not be viewed as providing a set of "validated" models. Rather, the goal should be obtaining sufficient confidence that the models are able to simulate the behavior of the real system to accomplish the regulatory purpose. Thus, the regulatory focus should be on (1) well-defined problems that test key processes, with less concern placed on the type and location of the specific media involved in a given experiment, and (2) site-specific application of the models to the proposed repository system. An example of a well-defined problem that tests a key process can be found in experiments conducted at Harwell Laboratory [Bourke and others, 1990] which consisted of clay plugs in which transport of a solute through the plug was measured. The key process that was assumed to be occurring was diffusion. Therefore, this experiment could be used to build or retract confidence in the application of Fick's second law to describe diffusion in a porous medium.

The final point to make about the definitions of validation is that absolute proof that models are perfect representations of reality is not required. Instead, the definitions indicate only that assurance be provided that the models are *adequate* representations of the real system. Defining what is "adequate" will, in the end, be a subjective decision made by the regulator. A specific criterion that defines "adequate" is beyond the scope of this report. However, this decision should be based on

1. Whether or not the types of validation tests are relevant to the intended use of the model;

2. How well the models were able to simulate the validation tests;

3. How many validation tests are sufficient before the models can be applied to a particular site; and

4. How well the site-specific information conforms with the model's description of the site.

It cannot be overemphasized that model validation is a site-specific issue based on the intended use of the model. For this report, the intended use of the models is assumed to be assessing compliance with regulatory requirements for a HLW repository. Although the ultimate decision on the adequacy of the model for the regulatory purpose will be, to a large degree, subjective and based on an acceptable level of uncertainty, emphasis should be on a rigorous development of the validation process. Validation information that is given to decision makers should be as all inclusive as possible and follow a logical systematic approach.

3.0 NEED FOR VALIDATION

The need for model validation in the U.S. HLW program arises from at least two sources. First, it is stated explicitly in 10 CFR Part 60.21(c)(1)(ii)(F) that "Analyses and models that will be used to predict future conditions and changes in the geologic setting shall be supported by using an appropriate combination of such methods as field tests, in-situ tests, laboratory tests which are representative of field conditions, monitoring data, and natural analogue studies." Second, there is legal precedent establishing the need for validation. The issue of validation was the basis for the decision in a court case involving the State of Ohio and the Environmental Protection Agency (EPA) [23 ERC 2091, Sixth Circuit, 1986]. In that case, the U.S. Court of Appeals ruled that EPA had acted arbitrarily in using the CRSTER computer code [EPA, 1977] as a basis for establishing limitations on sulfur dioxide emissions from two electric utility plants. The Court decided that the EPA had failed to establish the accuracy or trustworthiness of the model as compared with the actual discharge from the plants. More specifically, the Court stated that "no on-site study has been performed on the CRSTER model...no one has tested the model or cross-checked its predictions against reality at the locations of the company's power plants." In this case, the regulatory purpose was to establish limitations on sulfur dioxide emissions at the specific power plants, but the model used for this purpose was not compared to measured emissions from these plants. Therefore, the adequacy of the model for the specific purpose at the specific site was not demonstrated (i.e., site-specific validation of the model was not performed).

4.0 APPROACH TO VALIDATION

Given enough time and resources, it may be possible that all of the models used to assess the performance of a HLW repository could be compared to site-specific data. However, limitations in time and resources, as well as the possibility of compromising a site's integrity by extensive site characterization, leads to an alternative approach to validation. Foremost, these limitations lead to the use of as many relevant experiments as possible to test the models, and, therefore, build confidence in the models for the regulatory purpose. Hence, a validation approach should include the use of so-called "generic" validation experiments, as well as experiments performed at the proposed repository location (i.e., site specific). Examples of generic validation experiments would be experiments that test Darcy's law in several different media; thus, building confidence in transferring the model to site-specific conditions. Obviously, testing Darcy's law in the porous medium and ground-water found at the site would build the most confidence in using Darcy's law, but if this is not possible, generic validation experiments become necessary. In general, both generic and site-specific experiments will include laboratory tests, field tests, and natural analogues [Davis and others, 1990]. The usefulness and limitations of each of these tests for the model validation process is discussed in the following sections.

4.1. Use of Laboratory Experiments

Laboratory experiments are useful in testing the processes controlling the behavior of the repository system because (1) they are performed in a controlled environment that minimizes uncertainty in initial and boundary conditions, and (2) the experiments can be performed on samples that exhibit relatively little geometric variability (i.e., homogeneous). However, the use of laboratory experiments in validation efforts is limited due to (1) the inability to perform tests on either long time scales or large spatial scales required for assessing the performance of a HLW repository, (2) the difficulty in testing coupled processes, and (3) the possibility that the systems used are not representative of *in situ* conditions (e.g., samples damaged in collection, not enough samples collected to characterize spatial variability, laboratory conditions not equivalent to field conditions which may produce phenomena that does not actually occur *in situ*). Examples of laboratory experiments that may be used for model validation are the clay diffusion experiments conducted at Harwell Laboratory [Bourke and others, 1990] and experiments of uranium migration in crystalline bore cores performed in Switzerland [Bischoff and others, 1987].

4.2. Use of Field Experiments

Field experiments overcome, to a degree, the problem of representativeness of data and the spatial-scale problem that plague laboratory experiments. To a certain extent, field experiments can be direct surrogates of repository performance (e.g., field heater tests and tracer tests). However, the usefulness of field experiments is limited by uncertainties in initial and boundary conditions and, to a large degree, by the possible conceptual misunderstanding of field conditions. Examples of field experiments relevant to model validation are tracer experiments in a fracture zone at the Finnsjon research area in

Sweden [Gustavsson and Klockars, 1984] and flow and tracer experiments in crystalline rock at the Stripa mine [Abelin and others, 1985].

4.3. Use of Natural Analogues

In some sense, nature could be considered to have initiated experiments that could be used for validation. Transport of radionuclides from uranium deposits and transport and deposition of minerals along fractures are a few examples. These "experiments" have the advantage of having taken place on temporal and spatial scales that are comparable to HLW repository system scales. In addition, coupled processes are often involved that are difficult to produce in either the laboratory or the field. Uncertainty in initial conditions, boundary conditions, and the temporal evolution of the physical system, however, limit the usefulness of natural analogues in validating models. Some examples of natural analog studies are uranium migration at hydrothermal veins near Marysvale, Utah [Shea, 1984] and the natural ore body site at the Alligator Rivers area in Australia [Airey, 1984]. As discussed above, using natural analogues for model validation is not trivial; therefore, the reader is referred to Chapman and others [1984] for a more detailed discussion on natural analogues and their use in model validation.

5.0 APPROACH TO COMPARING MODEL PREDICTIONS WITH EXPERIMENTAL RESULTS

The following sections outline a generic approach to comparing model predictions with experimental results that is consistent with the philosophy discussed in Section 1 through Section 4. Salient features of this philosophy consist of the following: (1) due to the relevant time and space scales, models that are used to assess the performance of a HLW repository can never be validated; therefore, (2) validation is a process that consists of building confidence in models and not providing "validated" models; in this context, (3) model validation includes comparisons to "reality," however, adequacy for the given purpose (regulatory decision) is the overall goal; (4) comparisons to "reality" consist of comparing model predictions against laboratory and field experiments, and natural analogues; and (5) a model can only be "invalid" or "not invalid" based on the null hypothesis concept; however, some confidence is provided for in a "not invalid" model. The steps of the proposed approach are:

1. Definitions and prioritization of models for the validation process;

2. Identification and definition of relevant experiments;

3. Definition of performance measures that are based on the intended use of the model;

4. Quantification of the uncertainty associated with the input data and the data available for comparison with the model output;

5. Definition of acceptance criteria or acceptable model error based on regulatory requirements and uncertainty in experimental results;

6. Simulation of the experiment;

7. Experimentation; and

8. Evaluation of model results based on acceptance criteria.

Each on of these steps will be discussed in detail in the following sections.

5.1. Definition and Prioritization of Models

The licensing of a HLW repository requires that certain performance standards be met. The regulations do not explicitly provide specifications as to what, if any, models must be used; nor are there unique models for a given HLW application. On the contrary, many models exist that claim to simulate some aspect of a repository system. The choice of which models to use is up to the license applicant and the examination of the applicability of these models up to the regulator. Therefore, mapping between the performance standards and models that could be used to evaluate the repository system is the first step in the model validation process. This mapping involves defining a strategy for demonstrating compliance with a given standard and then developing conceptual models; choosing, developing, or modifying a computer code to implement the conceptual model; and obtaining the data required by the model. A conceptual model is the combination of all of the assumptions about the repository system that are required to adequately simulate the behavior of the system [Davis and others, 1990; Parson and others, 1991]. These assumptions are developed based on the real site and corresponding data. A mathematical model is a numerical expression of the conceptual model. It consists of a set of equations that describe the initial and boundary conditions, the governing processes and the solution of the equations. The mathematical model may or may not be implemented in a computer code. As stated previously, the combination of the conceptual model, mathematical model, computer code, and associated input data is what is herein referred to as a model. Once the models are chosen they can be tested against the relevant experiments.

Limitations of resources and time, and the possibility of compromising a site's integrity by extensive site characterization, do not permit testing of all possible models required in HLW performance assessments. One possible approach to deciding the priorities of which models to test first would be to follow the strategy given by Price and others [1990] on the review of performance assessment models. That strategy focuses first on processes that could directly lead to a release of radionuclides and proceeds to processes that reduce the chance that radionuclides would be released. Following a similar strategy, model validation studies could be forced to test the most important models first.

5.2. Identification and/or Definition of Relevant Experiments

Once the required models are identified, a combination of laboratory, field, and natural analog experiments, as discussed in Section 4.0, should be identified that test the range of expected repository conditions and processes that may occur under those conditions (both current and future). It is likely that experiments exist that test many of the expected processes (e.g., ground-water advection, solute diffusion, solute sorption). Therefore, experiments should be performed that test the remaining processes or conditions (e.g., coupled heat and advection, coupled liquid and gas-phase transport) not covered with existing experiments.

It cannot be overemphasized that the chosen experiments should be relevant to repository performance irrespective of the model's reported features. In other words, model purpose should be the focus of validation efforts, not features of the model. For example, if a model is able to simulate transient behavior, but steady-state analysis is appropriate for the intended use of the model (i.e., simulating repository performance), effort should not be expended on model validation of the transient feature. Too many past validation efforts (experiments and modeling) have not addressed licensing requirements but have focused instead on testing features of a given model. In fact many "generic" validation experiments have tested models or parts of models that will never be used to assess compliance with the relevant regulations. The pitfalls of such an approach go beyond unwise use of resources. First, the potential exists to develop false confidence in the model because the experiment is not relevant. Second, of equal importance, is the possibility of invalidating a model that is adequate for the purpose of assessing repository performance, but is unable to reproduce results of an experiment that tests conditions not found in a repository environment. To reiterate, this is not a question of whether the model is scientifically correct for all conditions but, rather, is the model adequate for the desired purpose (simulating anticipated repository conditions).

A point needs to be made here concerning experiments that have been performed prior to the validation effort. First, and perhaps most important, there is a great tendency to turn the validation effort into a calibration effort. This is because the data describing the results of the experiment are available prior to, during, and following the modeling effort. Thus, the modeler has a tendency to fit (or calibrate) the model results to the experimental results instead of using input data determined, ideally, independently from the experiment to *predict* the experimental results. Nevertheless, this type of an effort (i.e., calibration) affords some degree of confidence in the model if the results agree well. However, calibration by itself is not validation because the input parameters for the model are found based on the output of the experiments. If parameters cannot be measured independently, the experiment should be designed so that results of one experiment could be used to calibrate the input data and predict a subsequent experiment under different conditions.

Another consideration is that a "reasonable" fit can be obtained with many different models. Hence, designing experiments that can distinguish between models becomes important. This design may consist of an experiment that could be conducted under conditions where different model results could be discerned (e.g., a matrix-diffusion model is indistinguishable from a convection-only model for relatively large ground-water velocities, but at relatively small velocities the results are distinguishable). The reason that these problems exist is not a criticism of the experimental program, but is a result of the original purpose of the experiment. Namely, most past experiments were not specifically designed for validation purposes. Thus, it is likely that not all of the information (e.g., independently measured parameters) necessary for model validation was obtained or the experiment was not designed to be able to be performed again under different conditions. For the case of natural analogues, it is not possible, obviously, to design the experiment so that it can be conducted again. Ideally, the validation effort would rely only on specific laboratory and field experiments that are part of the repository program. However, this is not possible given the limited resources and time.

5.3. Definition of Performance Measures that are Based on the Intended Use of the Model

In order to judge the performance of the model relative to the experimental results, some representative measure(s) of the system response must be defined. A performance measure must be a quantity that is of regulatory interest or directly related to a quantity of regulatory interest. For the licensing of a HLW repository in the United States, the performance measures of regulatory interest are concentrations of contaminants, integrated quantities of contaminants, or travel time of contaminants through the geosphere. Regulatory analyses require these measures to be predicted over distances of kilometers and times of 1,000's to 10,000's of years. Because experiments on these scales are not possible, validation studies must rely on indirect measures of repository performance. There are two types of indirect performance measures. First, there are performance measures that are directly related to regulatory requirements (e.g., concentration and ground-water velocity), but are not measured on the appropriate regulatory space and time scales. Second, there are performance measures that are not measured on the appropriate space and time scales *and* that are not directly related to regulatory requirements (e.g., pressure and moisture content distributions). These should only be used as a last resort because of the potential for misinterpretation of the results. For example, a model may not be able to reproduce a three-dimensional distribution of moisture content, but if it can predict regulatory performance measures of interest it may be determined adequate for the intended purpose. Again, the point is not that the model is scientifically incorrect, but rather, since the performance measure is the basis for deciding what is acceptable, a performance measure that is not related to the intended purpose should not be used and can be misleading.

5.4. Quantification of Uncertainty

The ability of a model to adequately predict the performance measures cannot be judged without consideration of the uncertainty of the input parameters and the accuracy of the experimental results. Therefore, any validation program should address these uncertainties. One way of addressing input parameter uncertainty is by assigning a probability distribution for each parameter. Ideally, this distribution would be based on repeated independent measurements (e.g., bulk density measurements, porosity measurements) of the input parameter, but for some parameters, the only information available is values from the literature. Unfortunately, in some cases this may produce ranges of model output that are so large that it is difficult to ascertain whether or not the model results agree with experimental results. Again, repeated experiments, either independent or with the validation experiment under different conditions, should be conducted to reduce data input uncertainty. Input data uncertainty is further discussed in sections 5.5.2. and 5.5.4 as it relates to defining an acceptance criterion.

There are several types of error that could be associated with the experimental data. These include data collection errors (e.g., instrument error, human error) and interpretation errors (e.g., fitting a Theis curve). Some types of errors are quantifiable while others can only be estimated subjectively by the experimentalists. In any case, the responsibility of quantifying the errors associated with input parameters and experimental results lies with the experimentalists and not with the modelers. Therefore, when planning experiments for a validation program, the experimentalists should be aware of this requirement. Uncertainty in the experimental data is further discussed as it relates to defining an acceptance criterion in sections 5.5.1 and 5.5.4.

5.5. Definition of Acceptance Criteria

This is one of the most difficult steps in the validation process because the question of the adequacy of the model predictions relative to the experimental results is ultimately subjective. On one extreme, when the basis for comparison between model and experimental results is visual, it becomes very subjective as to what is "good enough." On the other extreme, even if a systematic approach is used to analyze the model error and present it in several different ways, in the end some acceptance criterion must be established, the level of which will be determined by subjective expert judgments [Bonano and others, 1990].

5.5.1. Experimental Measurements

In judging the acceptability of model results, the uncertainty in experimental results should be taken into account, as mentioned in Section 5.4. That is, the model can only be judged relative to the accuracy of the measurements. Accounting for errors in the experimental results can be accomplished directly by defining acceptance limits which correspond to a band defined by the experimental measurements, plus and minus their associated error.

5.5.2. Data Input

Accounting for the uncertainty in input parameters is more difficult than accounting for measurement errors in the experimental results, as mentioned in Section 5.4. To illustrate this difficulty, consider the following two extremes. First, the input parameters could be known with complete certainty. Given that the model is an accurate representation of the real system (i.e., the conceptual, mathematical, and computerized aspects of the model are "valid"), then the model results should agree with the experimental results within the accuracy of the experimental measurement error. However, if the model does not agree with the experimental results within the experimental error band, the model is "invalid" for that experiment. Second, consider the other extreme, that is, the input parameters are completely uncertain (i.e., unknown). This situation can occur when a particular parameter is not measured during an experiment. In this case, the modeler is free to assign any value to this parameter in an attempt to obtain agreement between model and experimental results (i.e., model calibration, as discussed in Section 5.2). In the event that the modeler is unable to obtain agreement in this manner, the model is "invalid" for that experiment. Normally, however, the modeler is able to achieve some degree of agreement between the model and the experimental results. This does not mean that the model is "valid"; it only indicates that the model is "not invalid" over the range of that experiment. Thus, uncertainty in the model input must be taken into account, but the judgment about the acceptability of the model should be tempered by this uncertainty. In other words, the more uncertain the data are, the more difficult it is to conclude that the model is acceptable.

5.5.3. Model Structure

In addition to the data uncertainty described above, the other main source of uncertainty is in the model structure. The model structure is the inherent structure of the conceptual, mathematical, and computerized portion of the overall model; that is, all aspects of the model except the input data. Model-structure uncertainty arises from an incomplete knowledge of the driving processes, a limited knowledge of complex natural geometries, and mathematical and computational limitations given the current state of the art.

5.5.4. Acceptance Criteria

Consideration of these two types of uncertainty, model structure and model input data, leads to the logical definition of at least two acceptance criteria for a given case. The first one is a measure of the accuracy of the model input parameters relative to the experimental results, while the second is a measure of the adequacy of the model structure in describing the system behavior. To illustrate the two types of criteria consider a simple tracer test through a column with a steady-state, uniform velocity field and a constant inlet concentration. In this example, the conceptual model to be tested is transport of a soluble species in a homogeneous, isotropic porous medium, the behavior of which is assumed to be governed by the classical convective-dispersion equation and the performance measure chosen is the concentration breakthrough curve.

Accuracy of model input. To elucidate the criterion used to judge the adequacy of the model input data, assume that the underlying model structure is correct. For the example described above, this means that the model and experimental results both display the classical S-shaped concentration breakthrough curve. Now, consider the possibility that the model predicts that the contaminant arrives earlier than the experiments indicate (see part a of Figure 5.1). Depending on how close the two curves are, the model results could still be acceptable. The proposed acceptance criterion is based on a combination of the distance between the curves, the uncertainty in input values, and the uncertainty in experimental results. Given these results, several possibilities arise.

First, it is possible that there is no overlap between the model-predicted values and the experimental results, taking into account the uncertainty in the experimental results (see part b of Figure 5.1) regardless of what combinations of model input parameters are used. In this case, the model is in error and this error arises due to incomplete knowledge of the values of the input parameters. If this happens, the experimentalists should attempt to make additional parameter measurements. The next possible condition for this acceptance criterion is that the model results agree with the experimental results (see part c of Figure 5.1). That is, some combination of input parameters results in model predictions that lie within the band created by the plotting

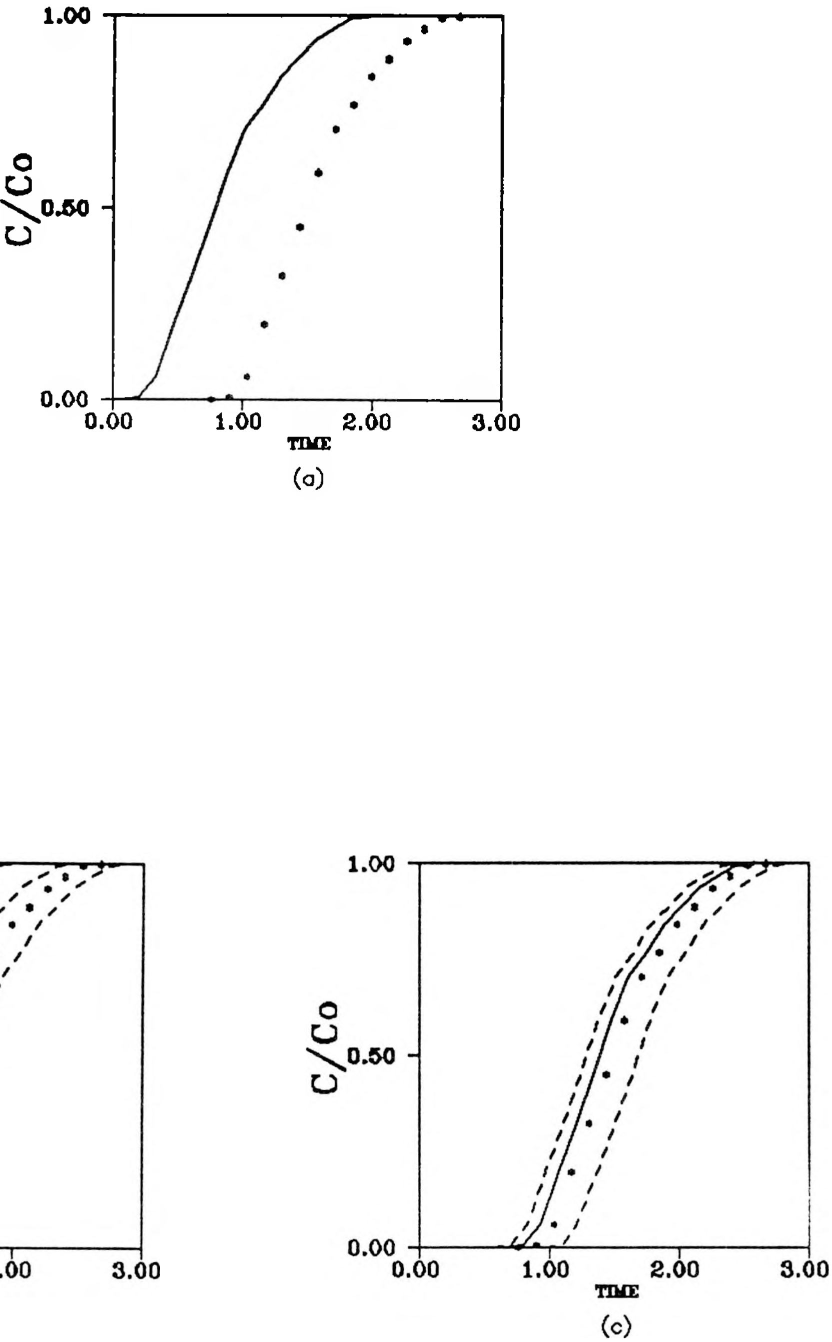

Figure 5.1. Column tracer experiment: hypothetical experimental and model results, (a) model predicts earlier breakthrough than experiment, (b) no overlap between model and experiment, (c) overlap between model and experiment.

of the experimental results and the associated experimental error. Being consistent with the null hypothesis concept presented in Section 2.0, for this case, one can only state that the model is "not invalid." However, confidence in the model is only obtained when the model is found to be "not invalid" over a wide *range* of experimental conditions. For example, the hypothetical tracer test would have to be repeated under different experimental conditions (for instance, the experiment would have to be repeated under a range of imposed velocities). To further illustrate this point, consider a model for tracer movement that assumes solute retardation can be represented with a constant retardation factor and, implicitly, that this relationship is applicable for all conditions (e.g., ground-water velocities). Conceivably, the modeler could find a value of the retardation factor that allowed the model to reproduce the experimental results (i.e., the concentration breakthrough curve for one steady-state velocity field). However, if the retardation factor was actually a function of velocity, the model would be "invalid" for all velocities other than the one used in the experiment.

Adequacy of model structure. A second acceptance criterion arises out of the need to determine whether or not the model structure (i.e., the underlying conceptual, mathematical, and computer model) is adequate. This criterion is based on the concept that the model results will have a unique form, regardless of the model input. For the example described above, the model output is always the classical S-shaped concentration breakthrough curve. If this equation is an adequate representation of the physics governing a particular experiment, then the experimental results should be of the S-shaped form. Deviations from this form indicate an incorrect model structure. For example, the tracer test described above could be affected by diffusion of tracer into dead-end pores. The experimental results, in this case, would display a concentration breakthrough curve which falls underneath the classical S-shaped curve at late times. This phenomenon of dead-end pore diffusion was not included in the model and the acceptance criterion should be designed to test for the differences it produces. One possible approach is to start with the "best fit" model obtained in the data-input uncertainty analysis described above. That is, start with the combination of data input that results in the closest fit to the experimental results. Using the best fit results as the representation of the behavior of the model, the approach could be to search for systematic differences between the model results and the experimental results. The basis for this is the assumption that random errors about the model results could be caused by measurement error but systematic errors result from inherent errors in the model structure. This search could be accomplished by subtracting the model results from the experimental results and testing these so-called residuals for a systematic trend. Thus, if the residuals do not reveal any detectable trend, the model adequately represents the experimental results and the model structure is acceptable. On the other hand, the model structure is in error if a trend exists in the residuals.

5.6. Simulation of the Experiment

Simulation of the experiment may require the use of a computer code depending on the complexity of the mathematical model. Most of the HLW performance assessment models used are so numerically intensive that a computer code is the only reasonable way to implement them. The calculations should include propagation of the uncertainty of the input data. Several uncertainty analysis techniques are available for this purpose [Zimmerman and others, 1990; Doctor, 1989]. One popular method is to use a Monte Carlo approach based on the Latin Hypercube Sampling (LHS) scheme [Iman and Shortencarier, 1984]. Using LHS, one can insure that the entire range of parameters are tested. However, it does not guarantee that the best fit model will be obtained. Inverse techniques do provide a best fit but generally do not provide information about other combinations of parameters that could work equally well. When simulating experiments for model validation, a serious attempt should always be made to simulate the experiments without reliance on or knowledge of the experimental results. This helps prevent biases in the modeling effort and, therefore, provides for legitimacy of the model results.

5.7. Experimentation

As discussed in Section 5.6, for model validation, the field or laboratory experiment should follow the model simulations to assure that the modeling effort is not simply a calibration effort based on the experimental results (i.e., biased). For most past cases, laboratory and field experiments were not conducted after the modeling effort. Again, the reason for this can be traced back to the original purpose of the experiment which was usually not related specifically to model validation. For natural analogues it is not possible to conduct the experiment after the modeling, however, obtaining the data after the modeling exercise is possible.

5.8 Evaluation of Model Results based on the Acceptance Criteria

In this step, the performance measure (for example, radionuclide concentrations) predicted by the model is compared to the experimental results using the acceptance criteria defined above as the measures of fitness. This allows one to conclude whether or not the model structure is correct and whether or not the model input data have been adequately estimated. In the event that the model structure and the input data are adequate, two questions remain. First, would the same model be able to adequately predict different experimental conditions and, second, are other model structures (conceptual models) also able to adequately simulate the experimental results. Both of these questions can only be answered with new experiments under different conditions. Understanding the differences in conceptual models should allow the modelers to recommend experiments that can only be satisfactorily simulated by one of the models.

Comparison of model predictions and experimental results may lead one to conclude that the input data were not adequately estimated. Again, the modeler then should be able to provide the experimentalist with a list of the desired data, including some indication as to which data are most important. The most important data could be determined by using sensitivity analysis of the model results.

Finally, comparison of model predictions and experimental results may lead to the conclusion that the model structure is inadequate for describing the experiment. The modeler would then have to propose a new model structure and repeat the simulations and model comparisons.

6.0 SITE-SPECIFIC MODEL VALIDATION

The approach outlined in Section 5.1 deals with experiments that test only certain models or parts of models and generally over relatively small spatial and temporal scales. However, the site-specific repository performance assessments that are required for licensing will be produced using a wide variety of models. As stated previously, this system of models cannot be directly tested because they predict conditions for 1,000's of years over scales of kilometers. While these models cannot be directly tested over these scales, certain site-specific factors can be evaluated to gain confidence in using the models to simulate repository performance over these scales. These factors are outlined below.

6.1. Agreement of the Model with Site-Specific Information

At a minimum the model input data must be site-specific. However, information other than input data is available to check the adequacy of the model for the intended purpose. Consider a ground-water flow model, for example. Not only should the model be based on site-specific hydraulic conductivities, but the model results should agree with other site-specific hydrologic information such as hydraulic heads, ground-water chemistry, and isotopic ages of ground-water. Questions will remain, however, as to the sufficiency of the data used for comparison and the degree to which the model must be consistent with other site information. In addition, the check for consistency generally can only be based on comparison with current conditions. Repository conditions (both natural and man-made) may change significantly over the time of interest for regulatory compliance (i.e., 10,000 years) which may lead one to question the model's predictive capability under conditions other than the current ones. Thus, a major effort should be the identification of sites similar to the repository location that are currently under conditions different from the repository site so that the adequacy of the models under possible future conditions can be evaluated. For example, it may be possible to find a site with similar geology to the repository site but that is currently under different (e.g., much wetter) climatic conditions.

6.2. Justification of Assumptions

The foundation of any model is its assumptions, both implicit and explicit. Therefore, considerable attention should be paid to the assumptions that are invoked in simulating the performance of the repository system and the basis for those assumptions. If the generic validation tests had covered all possible conditions of model use, then this task would involve only choosing those assumptions used with experiments that were identical to repository conditions. For example, if generic validation experiments established that Darcy's law was applicable for all types of porous media, assuming ground-water Reynolds numbers less than one, one would only have to establish that Reynolds numbers less than one existed at the repository site. Unfortunately, all inclusive experiments of this type are not possible and determining which assumptions are transferrable from experimental conditions to repository conditions is difficult, if not impossible, since the future state of the repository is not known with certainty. However, given the problem at hand, each assumption should be justified to the extent possible with site-specific information, site-specific validation experiments, and generic validation experiments. The adequacy of untested assumptions will have to be established based on expert judgments [Bonano and Cranwell, 1988; Bonano and others, 1990].

6.3. Multiple Conceptual Models

Conceptual models have generally been developed based on a "single" interpretation of existing site-specific data, and where data were lacking, using expert judgments. However, no matter how well characterized a site may be, multiple conceptual models are possible that are all consistent with available data. In fact, the use of multiple conceptual models in HLW repository performance assessments should be encouraged to give some assurance that the results encompass possible system behavior. Care should be taken, however, that the necessary data were gathered during site characterization to exercise the models, as well as to include the different conceptual models in a validation program. Validation experiments that are designed for different conditions (e.g., large range of ground-water fluxes) can also be used to distinguish between proposed alternative conceptual models. For example, a large fractured block experiment conducted under different ground-water flux conditions could be used to distinguish between a dual-continuum flow model and an equivalent-porous-medium flow model.

7.0 CONCLUSIONS

HLW performance assessment models cannot be proven to be valid due to the temporal and spatial scales of regulatory concern. However, given the problem at hand (nuclear waste disposal), confidence in these models can be gained through testing model performance against a combination of laboratory and field experiments, and natural analogues, as well as providing evidence that the models are consistent with site-specific information. An attempt should also be made to include all equally plausible conceptual models that are consistent with site-specific data in the final assessment and in a validation program. When comparing model predictions to experimental data, confidence arises by showing that the models are "not invalid" over a wide range of conditions and acknowledges that "validated" models used for performance assessment are not possible. A logical approach for comparing model results with experimental data is testing model input data separately from model structure.

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