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ABSTRACT

The safety assessment of underground disposal of nuclear or toxic wastes requires the use of models. Such models need to be validated to ensure, as much as possible, that they are a good representation of the actual processes occurring in the real system. In this paper an attempt is made to take a broad view by reviewing step by step the modeling process and bringing out the need for validating every step of this process. Thus model validation includes not only comparison of modeling results with data from selected experiments, but also evaluation of procedures for the construction of conceptual models and calculational models as well as methodologies for studying data and parameter correlation. The need for advancing basic scientific knowledge in related fields, for multiple assessment groups, and for presenting our modeling efforts in open literature for public scrutiny is also emphasized.

Introduction

The assessment of long-term safety of underground disposal of nuclear and toxic wastes demands much more of the scientists and engineers and their model predictions than the safety evaluation of many civil constructions such as dams, or resource evaluation of many petroleum or geothermal reservoirs. The extra demands are mainly due to two factors:

(a) The safety assessment usually involves the estimation of low concentrations (low probabilities) of solutes transported over kilometers for thousands of years into the future.

(b) Data characterizing the rock mass at the disposal site are necessarily sparse, since too many data-collecting boreholes may adversely impact the integrity of the rock mass. Thus, there may be large uncertainties in our knowledge of the geometric structures, boundary conditions and relevant processes present at the site.

There is much interest and concern in many countries with toxic and nuclear waste management problems on the question of whether a model used in a safety assessment program is valid in making appropriate long-term predictions. In the area of toxic waste management, a number of authors (Moran and Mezgar, 1982; Huyakorn et al, 1984; van der Heijde et al, 1985; van der Heijde, 1987; Beljin, 1988; and others) have addressed this question. There is also a move to establish a groundwater research data center for the validation of subsurface flow and transport models (Miller and van der Heijde, 1988, and van der Heijde et al, 1989). In the area of nuclear waste management, a number of recent international cooperative projects, e.g., Hydrocoin (Grundfelt, 1989; Grundfelt et al, 1990), Intraval (Andersson, 1989; Nicholson, 1990), Stripa (Herbert et al, 1990), Chemval (Broyd, et al, 1990), Biomovs (SSI, 1990), and others, have been devoted to the validation of models. Model validation was also extensively discussed in number of symposia, such as GEOVAL87 (1987) and GEOVAL90 (1990). Some general comments on model validation were given by Tsang (1987) who pointed out the need to differentiate between model structures and model processes. Additionally, there is a wealth of literature on validation in the field of system engineering and operations research which may be useful for our consideration. Examples include Balci (1988, 1989), Balci and Sargent (1984), Gass (1983), Gass and Thompson (1980), Oren (1981), Sargent (1984, 1988), Schruben (1980) and Zeigler (1976).

Up to now most validation efforts on the safety of geological disposal involve simply a comparison of modeling results against field data. The present paper presents a broader view, that, to validate models that will be used for long-term predictions, validation needs to be carried out at every step of the modeling process. We shall begin by giving a few definitions to establish common understanding of several key terms for the subsequent part of the paper. Then we shall describe a detailed step-by-step process for model predictions. The following section will discuss possible validation issues associated with steps of the modeling process. Three miscellaneous, through important, remarks conclude the paper.

A Few Definitions and Comments

There have been a number of definitions of model validation. The International Atomic Energy Agency (IAEA, 1982) defines validation as follows: "A conceptual model and the computer code derived from it are validated when it is confirmed that the conceptual model and the computer code provide a good representation of the actual processes occurring in the real system." Schlesinger et al. (1979) defined validation as meaning "substantiation that a computerized model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model."

In the context of these definitions of model validation we shall understand a model as a combination of (a) conceptual model and (b) computer code, with the relevant model parameters, which are derived from field and laboratory data and information. Only with the combination of these elements is it possible to perform modeling studies whose results may be used as a representation of the actual processes occurring in the real system.

A site-specific conceptual model consists of three main components: structure, processes, and boundary and "initial" conditions. "Structure" refers to the geometric structure of the system, such as stratigraphy, faults, heterogeneity, fracture density and lengths, and other geometric and geologic characteristics. "Processes" are physical and chemical phenomena such as buoyancy flow, colloidal transport, matrix diffusion, and dissolution and precipitation. "Boundary conditions" are constant or time-dependent conditions imposed on the boundaries of the model domain. "Initial conditions" are the physical and chemical conditions over the model domain at a particular instant of time. This is usually taken at the initial instant of time, though in general it can be any specified point in time. The three main components of a conceptual model is summarized in Figure 1. Both structure and boundary and initial conditions are site-specific and scale-dependent and usually appears in modeling study as calculational mesh designs and input data. Processes, on the other hand, are usually described by mathematical equations being solved in a computer code and can often be studied in the laboratory. In practice, there are often cases where they are intimately coupled.

A computer code is a calculational program that solves a given set of equations with given inputs by numerical manipulations. Computer codes are said to be certified, when the code is properly verified and properly documented. In other words, it is mathematically correct in the formulation and solution, and properly documented on its purpose, accuracy, required discretization and ranges of applicability. However, it is illogical to use the term "code validation," as some modelers have done, since "validation" questions the appropriateness of the mathematical equations and input data and conditions, which are assumed and taken for granted in a code.

Model calibration is the process by which certain unknown parameters to be used in applying a code are determined by comparing modeling results with available data, which the model is required to simulate. For safety assessment of nuclear waste repositories, the models are expected to predict data for thousands of years into the future, and calibration is done to estimate parameters with short-term data. In this paper we assume this kind of calibration to be part of site characterization activities, where tests and analyses (which may well include modeling calculations) are done to determine the needed model parameters for assessment of repository safety for thousands of years.

Based on the above discussion it may be apparent that almost by definition one can never have a validated computer model without further qualifying phrases. In our view, a model, including the conceptualization and the code, can be said to be validated with respect to (a) a process or (b) a site-specific system. For (a), a process is first identified (e.g., buoyancy convective flow) and then conceptualized (e.g., as temperature-dependent density and viscosity) and coding is performed on this conceptualization. The model, composed of conceptualization and code, is then applied to a buoyancy experiment and its results compared with measurements. If the agreement is satisfactory then one can say that the model is validated with respect to this specific process. It is important to carry out model validation with respect to various processes, because it establishes our capability in predicting the effects of these individual processes that may occur at a site. This is indeed the subject of a number of current international projects.

For (b), a site-specific system is composed of a number of processes and the geometric structures, with boundary and initial conditions. It is an important and nontrivial problem to identify the presence of these processes and structures. Once they are identified, a model or group of models may be used to simulate the system and results can be compared with field observations. If successful, the group of models is said to be validated with respect to this particular site, within a range of applications determined by the range of field observations studied.

Hence, it is illogical to refer to a validated model in the generic sense. Rather, it can be stated that "a model is validated with respect to a given process," or that "a model or group of models are validated with respect for a given site." Ranges of applicability should be stated with these statements. Though model validation with respect to processes is an important subject currently under study by many groups, in what follows we shall only address model validation with respect to a given site.

The Modeling Process

In this section we shall itemize and discuss the steps in a site-specific model prediction calculation. We call this a modeling process, which is distinct from the physical and chemical processes referred to in the last section. There are alternative definitions of steps in a modeling process. We have chosen to define the process in broad steps that are appropriate for site-specific performance predictions thousands of years into the future.

The first step in the modeling process (see Table 1) is review and evaluation of available data. This is more than searching the data base to obtain numbers that we need for a given modeling calculation. A good modeler studies the complete data base to obtain as good as possible an overall picture of the site and relevant processes occurring there. For this, some preliminary calculations may be necessary. Of particular interest is an evaluation of data correlation. Data correlation is of two types. The first is spatial or temporal correlation. This is often studied by statistical methods. The second which may be of more importance is parameter correlation, which limits the range of values a parameter can have because of a chosen value of another parameter. For example, Wang and Narasimhan (1989) pointed out that there is such a correlation between the saturated conductivity and air-entry pressure (or radius) for the unsaturated zone at the Yucca Mountain site. Earlier studies have used too large a saturated conductivity value together with too small an air-entry radius value as inputs to a modeling calculation. Such combinations are physically impossible.

The second step is the development of a conceptual model and potential scenarios. This is to abstract the essence of the data base to construct the structure of the geometric model, to identify relevant physical and chemical processes involved in the system, and to determine appropriate boundary and "initial" conditions (Figure 1). Sometimes the data may be uncertain or even internally inconsistent and some subjective judgement will be required. The physical and chemical processes associated with the system with the boundary and "initial" conditions also define possible scenarios in time which also have to be identified and evaluated according to their probabilities of occurrence.

The establishment of performance criteria is the third step. This is related to "domain of applicability" or "range of application" in the definition of validation according to Schlesinger et al. (1979). Performance criteria are the quantities of interest that the model is asked to predict. There is the possibility that a performance criterion could be defined in such a way that the quantity of interest can never be predicted with sufficient accuracy because of intrinsic uncertainties in data. For example, in a highly heterogeneous fractured porous medium, it is probably impossible to predict tracer concentration at a particular point in space and time. Thus one has to modify the performance criterion to something more plausible yet still acceptable for the problem at hand. In the same example, instead of requiring the prediction of a point value of tracer concentration, we can ask for an integrated tracer concentration over a period of time and region of space (Tsang, 1989a, 1989b). In safety assessment of long-term waste disposal, this is perhaps the appropriate quantity of interest..

The fourth step of the modeling process is the construction of calculational models and the determination of the associated lumped parameters. Conceptual models are usually complex and are by definition three-dimensional so that simplification is always needed before modeling can proceed. We call these simplified models the calculational models. Often it is convenient that different simplification procedures are used for the calculation of different quantities of interest. Thus a very simple calculational model is perhaps needed for thermal field calculation, while finer features need to be added to calculate tracer transport. By lumped parameters we mean not only those parameter values averaged over spatial regions, but also those combining several more elementary parameters. For spatially lumped parameters, there needs to be much consideration how they should be defined especially in the case of strongly heterogeneous systems. I believe it is still an open question how to define properly scaled permeability and dispersivity for a medium with subregions of different flow and transport properties. An example of a lumped parameter incorporating elementary parameters is the relative permeability function for an unsaturated fractured porous medium, where it is shown (Pruess et al., 1990) that an equivalent porous medium with a specialized relative permeability function is adequate to calculate flow in the system, instead of the detailed parameters associated with liquid and gas flows in fracture networks and matrix blocks. The choice of calculational models and their associated lumped parameters is strongly dependent on the computer codes that are available or that can be developed in the near future. For example, if the code is able only to perform two-dimensional calculations, the calculational model would have to be two-dimensional.

After the decision on calculational models, calculations can proceed. Computer runs are made to yield tables of results and graphical outputs. There is a need to study the sensitivity of these results on parameter or data uncertainties. Many times, stochastic modeling techniques are used and results may then be given as probability distribution functions.

The next step is to understand and evaluate the calculational results. These results, including the estimated uncertainties, have to be evaluated according to the performance criteria. These uncertainties may arise not only from data uncertainties, but also from every step of the modeling process discussed above. For example, a particular choice of calculational model may introduce considerable uncertainties. One could ask the question, how well can a two-dimensional model simulate a three-dimensional system? Or, one could ask, is the conceptual model correct? Thus, results based on alternative conceptual and calculational models, will be studied. One may also want to consider redefining performance criteria to address more appropriate predictive quantities of interest in order to understand or reduce the uncertainties.

The outcome of the above evaluation step could be that the predictive results contain too many uncertainties. In that case one would define further information needs for new site investigations and measurements to be made to provide updates to step 1 and redo the modeling process with these new data. Thus the modeling process is an interactive or loop process.

The final outcome would be either that the predictive results with its uncertainties is satisfactory and a decision can be made, or new modeling calculations or new data (at reasonable cost and time) cannot reduce the uncertainties, and therefore the efforts should be terminated.

The Broad View of Model Validation

Since the goal of model validation is to ensure that modeling results provide a good representation of the actual processes occurring in the real system (IAEA, 1982), validation should be applied to every step of the modeling process as discussed above.

Thus for the first step of data review and evaluation, the methodologies of evaluation of data (spatial or temporal) correlation should be studied, understood and validated. This depends much on the scientific experience and knowledge of the personnel involved in the work and in the peer review process.

Construction of the conceptual model and evaluation of various possible scenarios requires much expertise and practice. One way to provide some confidence in this process is to involve more than one group of hydrogeologists, geochemists, geophysicists and geologists to perform this step. Cross-checking of the final results and understanding the differences between the outputs from the different groups may be extremely valuable.

The step of simplification of the complex conceptual models to calculational models and their associated lumped parameters has been often overlooked in model validation. It would be useful to put this on a proper scientific basis. Each modeling team should evaluate the uncertainties involved by alternative simplifications to arrive at alternative calculational models. Sensitivity of final results on the alternative models as well as on parameter uncertainties should also be studied.

Currently the most common validation approach used by many workers in this field involves the following. First a field or laboratory experiment is selected. Then the experimental conditions are specified, which include both the initial conditions and boundary conditions. Often not all boundary conditions are known. Then model computations are made and predictions are checked against field or laboratory data. However, there are other validation methods. Sargent (1984) presented the following list:

(1) *Event validity.* This represents an initial validation test of a qualitative nature, in which events of occurrences of the simulation model are compared with those of the real system.

(2) *Face validity.* This may be considered as part of peer review, involving asking people knowledgeable in the field whether the model is reasonable. The model flowchart may be checked for its correctness, and model input-output relationship may be checked for its reasonableness.

(3) *Traces.* The behavior of the different elements or entities of a model are traced or followed through the numerical model to determine if the logic and the program are correct and if the necessary accuracy is maintained.

(4) *Historical methods.* A historical method may consist of three steps: (a) examining the model's assumptions in theory, observations, general knowledge and intuition; (b) validating each of the model's assumptions, where possible, by empirically testing them; and (c) comparing the input-output relationship of the model to field behavior.

(5) *Internal validity.* This is particularly important in the validation of stochastic models or models with statistical inputs. Several realizations of a stochastic model are used to determine the amount of stochastic variability in the model. A high degree of variability may cause the model's results to be questionable and may require a redefinition of appropriate quantity of interest, i.e., appropriate performance measure.

(6) *Historical data validation.* If historical data exist for a given site, part of the data may be used to construct and calibrate the model and the remaining data are used to check against calculated results from the model.

(7) *Predictive validation.* The model is used to provide predictions for a given field or laboratory test and further measurements are made to check these predictions.

(8) *Turing tests.* This may also be considered a part of the peer review and is particularly important for stochastic models. Here people knowledgeable about the field are asked if they can discriminate between model output and field observations.

It is of interest to note that historical data validation and predictive validation are only two out of a number of validation methods. We should apply all the above list of validation methods, wherever possible, to all steps of the modeling process. For example, the methods of traces and face validity, though commonly known in operations research (Sargent, 1984; 1988), have been seldomly used up to now in our field. Often we depend on model developers and model users to ensure the correctness of model logic and accuracy. Very often, this is not adequate.

Need for Multiple Assessment Groups

As mentioned in the last section, some of the modeling steps, such as the design of conceptual models and the construction of calculational models, will be difficult to validate in a objective way, since their validation depends on the depth and breadth of scientific knowledge of the modelers involved. One approach for validation is the use of multiple assessment groups. Two or more groups studying the same geologic system independently may come up with different scenarios, different conceptual models and different simplifications in the construction of calculational models. Discussions among these groups will clarify the reasons for the differences and stimulate new considerations and better understanding of the system to be modeled. Thus, such interactions not only cross-verify each others' work, but also promote cross-fertilization to hopefully arrive at a more "valid" solution. We may define this multiple assessment group approach as one of the possible validation methods. Modeling results arrived at through the study and interaction of independent groups are more likely to be free from gross errors, and will probably have credibility among the scientific community and the public.

Multiple assessment groups do not necessarily imply multiple requirements of budgetary and personnel resources. First of all, the safety assessment modeling studies represent only a small budgetary component of the total cost of toxic and nuclear waste disposal. Secondly if budgetary and personnel resources are really a problem, the multiple-group approach can be applied only to the early steps of modeling where usual validation methods cannot be used easily. The later steps of carrying out detailed computations and presentation of results can be performed by one major group. International cooperation will also be helpful.

The multiple assessment group approach cannot be replaced by the expert peer review approach. Usually experts are requested to serve on a limited time period to study a problem, and their comments may focus on the technical procedures and methodologies used by the modelers involved. More likely than not they do not have time to study the primary site-specific data and come up with an independent view. Thus in most cases it is hard for them to become site-specific experts. On the other hand, the multiple assessment group approach allows each group to study and consider primary data in detail and develop the model unbiased by the views of other groups. Then interaction and discussions among the groups will be in depth with fruitful results. Some experiences of this nature have been found in the international cooperative projects such as Hydrocoin (Grundfelt, 1989; Grundfelt et al, 1990) and Intraval (Andersson, 1989; Nicholson, 1990).

Need for Basic Research and Public Scrutiny

If one examines the modeling steps and various validation methods as discussed above, one quickly comes to the realization that how well modeling results can predict future behavior of real systems depends very much on the state of our knowledge of various physical and chemical processes that take place in complex geological systems which can be characterized only in a limited way. It also depends on the state of field testing technologies and analysis methodologies. We should advance our state of knowledge and the art of measurement and modeling techniques by short-term laboratory and field experiments, long-term natural analog studies, as well as mathematical developments. Without proper understanding of physical and chemical processes and the system structure involved there could be no validation. A thorough understanding represents actually the major part of validation. Thus a percentage of our waste management effort should be devoted to such basic studies to add to the general geoscience state of knowledge and methodologies.

One of the best ways to draw on the reservoir of available knowledge is not only by the various validation methods indicated in the last section but also by having our modeling work published in the open literature. This should be done in parallel to the usual peer review panel process. Open-literature publications receive the benefits of public scrutiny. Sometimes an error may be pointed out by scientists from a different but related field of research. A study whose results are in the open literature examined by and maybe used by the general scientific community over a number of years has a much better chance of being free from gross errors. Eventually the decision if a model is valid is not made only by those doing the modeling studies. It is the general scientific community that will decide whether to accept the validity of models and whether they are used in the correct context.

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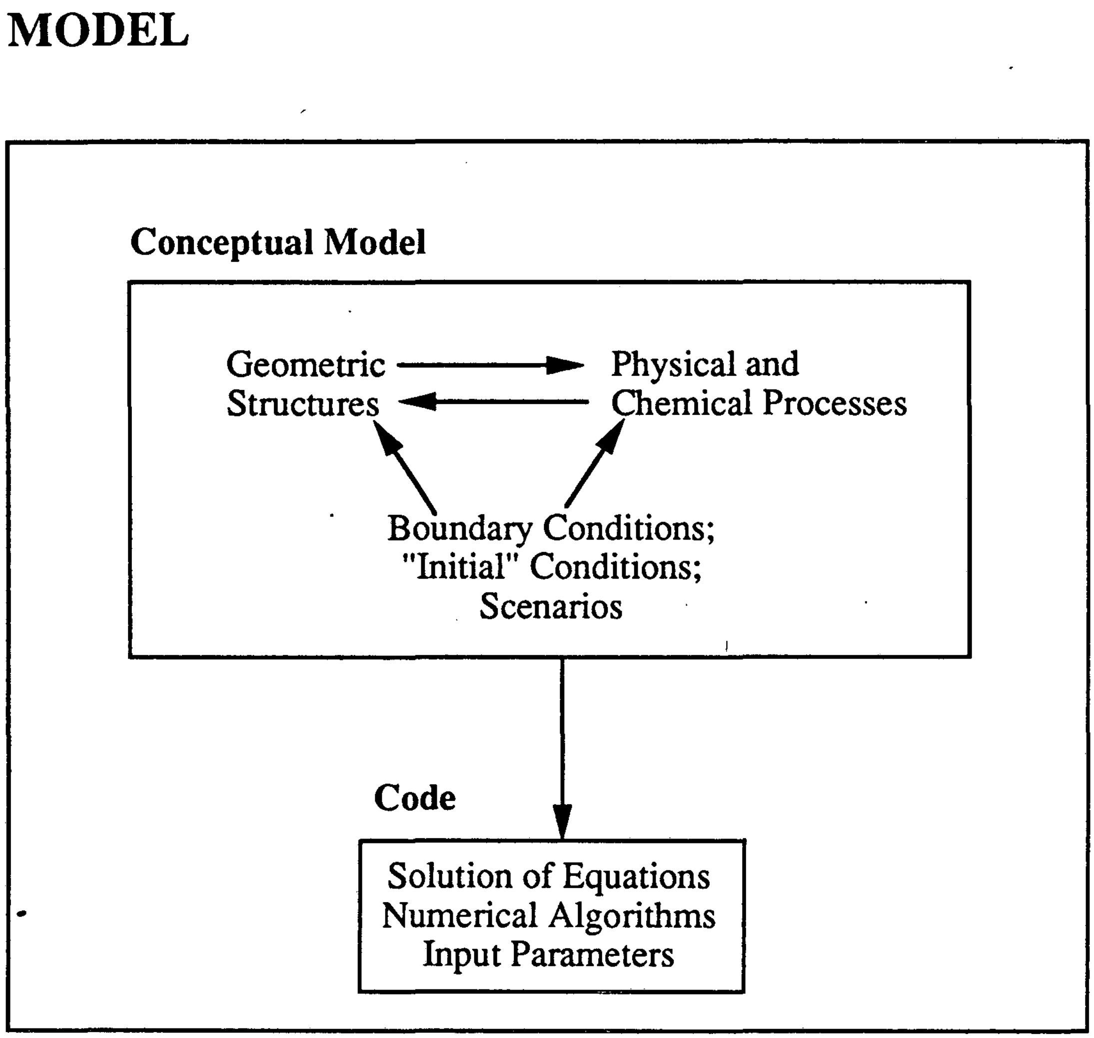

Figure 1. Schematic diagram relating model, conceptual model, and numerical code for site-specific modeling.

Table 1. Steps of the modeling process and their validation.

The Modeling Process	Examples of Issues Requiring Validation
1. Data Review and Evaluation	Spatial correlation and parameter correlation.
2. Conceptual Model and Scenarios; "Reasonable" Alternatives	Accuracy of conceptual model and probability of scenarios.
3. Performance Criteria	Appropriate choice of quantities of interest Are the criteria unnecessarily demanding?
4. Calculational Models and Lumped Parameters for all "reasonable" alternative conceptual models and scenarios	Simplification procedures and determination of lumped parameters from data.
5. Modeling Calculations, Sensitivity Studies, and Uncertainty Analysis	Uncertainties in data, in conceptual model and in calculational model choices.
6. Results Evaluation:	
(a) Uncertainly too large; Define new data needs; Design new site characterization activities:	GO TO STEP 1
• Feasible to perform further field studies, update data.	↑
• Not feasible within reasonable time and cost	→ STOP
(b) Results with estimated uncertainty good enough	→ INPUT TO DECISION MAKING