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C.-F. Tsang

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COMMENTS ON MODEL VALIDATION

Chin-Fu Tsang

Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94702 USA

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Earth Sciences Division
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University of California
Berkeley, California 94702 USA

ABSTRACT

The present paper points out the importance and usefulness of recognizing the separate roles of processes and geometric structures in predictive modeling of the performance of a nuclear waste repository or underground injection disposal of toxic wastes. Based on this a validation procedure is proposed. Furthermore, two stages and three elements of validation are described and discussed. Finally, comments are made on the choice of measurables to be used to compare modeling results and field data in the validation procedure.

INTRODUCTION

In the use of numerical models to predict the performance of a nuclear waste repository or the fate of toxic waste injected underground, there is much concern that the numerical models should have been properly validated. International projects such as INTRACOIN (1984, 1986) and HYDROCOIN (1987) were carried out mainly because of this concern. Some of these efforts were summarized by Andersson (1987). Model validation was also extensively discussed in a recent symposium (GEOVAL 87, 1987).

Numerical models have been used for predictive purposes in groundwater hydrology and in petroleum and geothermal reservoir engineering. However, in both these cases the requirements on predictive capability are relatively modest. In groundwater hydrology, one is mainly concerned with the availability of water

supply and management of water resources. In petroleum and geothermal reservoir engineering, one is mainly concerned with the available and extractable amount of energy resources. Predictions in both cases are expected to be made for a period less than 100 years. Usually adjustments in predictions are acceptable during the course of use or development. However, for the performance prediction of nuclear waste repositories one is concerned with solute transport over thousands of years.

For this reason in the case of geologic isolation of toxic or nuclear wastes, validation takes on increased importance and difficulties. There is need to consider slow processes that are significant over a time frame of hundreds or thousands of years. A carefully considered validation procedure is necessary. The present paper summarizes a number of considerations of this procedure.

First, a validation procedure is proposed and outlined. The importance and usefulness of differentiating between geometric structure and appropriate processes are pointed out. Next, two aspects, two stages and three elements of validation are presented. Then two comments on measurable observables will conclude the paper.

A Validation Procedure

A number of definitions for the term "validation" has been suggested. Perhaps the best definition is the one adopted by the International Atomic Energy Agency (IAEA, 1982), which states that:

> "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. Validation is thus carried out by comparison of calculations with field observations and experimental measurements.

Thus, in considering model validation it is useful to note a few important factors which are inherent to the problem of modeling physical and chemical processes in geologic formations. First of all, the model is no more than a conceptual picture of what the modeler constructs for the system, together with the corresponding mathematical equations and numerical solutions of these equations. The results depend strongly on how the inputs are designed and how they are used. Since

the conceptual picture can never be as detailed as the real system because of the lack of information and computer capability, the model is necessarily a simplification of reality. It is a good representation of the real system if the model is adequate to yield results for specific observables of interest, with the required accuracy and within a specified range of conditions. Thus, before embarking on a modeling exercise, we need to determine.

(a) What are the observables of interest,

(b) what is the the accuracy required for the prediction of these observables,

(c) the range of conditions for which the model is validated.

For example, the observables of interest could be point tracer concentration at a given time, or the integrated tracer output concentration over a spatial region and a time period of a few thousand years. The former depends on fine details of the system of fractures and channels in the geologic medium; we suspect no currently available model is able to give the correct predictions except under very special conditions. For the latter, however, methods may perhaps be developed to calculate the integrated quantities.

It is important to establish the range of applicability of "validated' models. We do not believe that a model can be developed that is valid for all situations. Defining the applicability ranges can perhaps help to avoid applications of the models to conditions for which they have not been validated.

In model processes in geologic media, it is useful to differentiate between processes and model structures. Model structures (Carrera and Neuman, 1986) can also be referred to as geometric structures. Processes are physical and chemical phenomena, such as buoyancy flow, colloidal transport, and dissolution and precipitation. Model structures represent geologic and geometric characteristics of the medium, such as faults, layering and heterogeneity. Processes can probably be studied in the laboratory and described by mathematical equations, whereas model structure are site- and scale-dependent and are part of the input data to the model. For a successful modeling study, one needs both the proper process identification (PI) and the proper model structure identification (MSI). Failure of matching modeling results with the field data could be due to errors in PI and/or MSI. Processes and model structure are approached quite differently. For example, models of processes can be validated generically, but models of

geometric structure are site-specific. In practice, there are often cases where processes and model structure are intimately correlated.

Figure 1 illustrates the discussions above. Ideally there should be an element in the model that can be used to suggest what further measurements are needed to improve the confidence level of the predictions. These further measurements are shown in the figure as network design (ND), which is the design of a network of measurement points with specificed time schedules to improve the model inputs. The procedure can be repeated or iterated (line connecting ND to Input to the figure) until one of the following two outcomes are reached:

(a) The prediction converges so that additional measurements do not result in a change in prediction, or

(b) the prediction does not converge and additional measurements are so expensive and time-consuming so that further work is not practical. In this case, we arrive at the "acceptable" results that the model predictions are not useful.

Two Aspects, Two Stages and Three Elements of Validation

The above discussions lead to some implications in regard to validation of performance prediction methods. These are summarized in Table I. The table indicates that there are two aspects associated with system performance, i.e., the appropriate processes and the geometric structure. By the latter, we also include the boundary and initial conditions. The table also emphasizes that there are two stages to arrive at validated performance predictions. The first stage involves system comprehension or basic understanding of the main features of the system (McCombie, et al., 1987). This should include the identification of appropriate processes and geometric structures as well as generic studies and research of their effects. Some of the current projects are projects in this stage. Once a basic understanding is obtained, the second stage involving a few sequential steps may be carried out. At the first step, the performance measures are selected. These are the "bottomline" quantities which have to be predicted in order to determine whether the performance is satisfactory or acceptable. Then an idealization or simplification of the in-situ geometric structures is carried out, and relevant and significant processes are identified and represented by appropriate mathematical formulation. To be able to do this implies that the first stage

concerning system comprehension has already been achieved. This step of idealization is probably always necessary because it is impossible to obtain data on all details of the system, and even if we have all the data, it would be impractical to perform calculations on all these details.

After simplification and idealization are done, then sample calculations for the particular site or bounding calculations can be carried out. One may remark here that the bounding calculations follow the step of idealization or simplification which in turn depends on system comprehension or basic understanding of the system. Thus, meaningful bounding calculations cannot be done without a basic knowledge of the geometric structure and processes present. Here the importance of the first stage in performance assessment is again emphasized. Following the bounding calculations in the second stage, sensitivity studies should be made and ranges of applicability determined. None of the bounding calculation results can be accepted without qualification. An awareness of the ranges of applicability is of great value.

Based on the above discussions, we would like to point out the need of three elements of validation as shown in Table I. The last element involving validation of predictions of a mathematical model on the responses of various processes in a system with given model structures is well known and accepted. What we are proposing here is the urgent need to validate the first two elements, i.e., the procedures for processes and structure identification and the procedures for simplification and conceptualization. To develop and validate (if possible) properly designed procedures for these two elements has been much overlooked and is an area of research that need more attention today.

Need to Establish Performance Issues for Validation

There have been a number of validation exercises that proceed from the selection of numerical codes and then, based on the capabilities of these codes, select laboratory or field data sets against which they will be validated. Sometimes, new laboratory or field experiments are performed specifically to obtain data that can be used to validate these code capabilities. We propose that it is more correct to proceed in the opposite way as follows. Without regard to available codes and their capabilities, let us consider what are the key issues in the performance of a nuclear waste repository or the fate of injected toxic wastes. Based

on these key issues, let us identify the relevant processes and geometric structures that are important. Then appropriate laboratory or field experiments are performed to obtain well-defined conditions and data. Finally, code developers have to come up with suitable codes and simplification methods to reproduce the results.

Comments on Measurables for Validations

Two comments will be briefly made here. First the usual observables that are commonly measured for validation studies involve solute concentration, salinity, temperature, liquid pressure and flow rates. For two-phase problems, one should also consider measuring gas flow velocities. Special tools may have to be developed for this. Another class of measurables we should consider are geophysical responses, such as seismic or electromagnetic signals. Some of these geophysical measurements may be very sensitive to changes in fracture apertures or changes in two-phase conditions. In saturated media, for example, a nuclear waste repository is filled with air during construction and waste emplacement. Thus, two-phase condition exists even in this case. Geophysical techniques for these purposes are still in an initial stage of development. However, we could hope that these geophysical measureables coupled with conventional measurements can be used to validate models.

The second comment is that the choice of observables used for validation purpose is most crucial. There are observables, such as point and instantaneous solute concentration field data, which is almost impossible for models to predict except in very simple systems. Perhaps the averaged solute concentration over a large region and over a period of time is more relevant an observable for determining the effectiveness of geologic isolation of nuclear or toxic wastes.

CONCLUSION

In this paper we have stressed the usefulness of separating processes and geometric structural effects in the validation of predictive modeling. Generally, we believe that this approach clarified a number of problems in validation procedures. A discussion of two stages and three elements for validation was given. The paper hopes to contribute to a better definition of the problems that lie before us.

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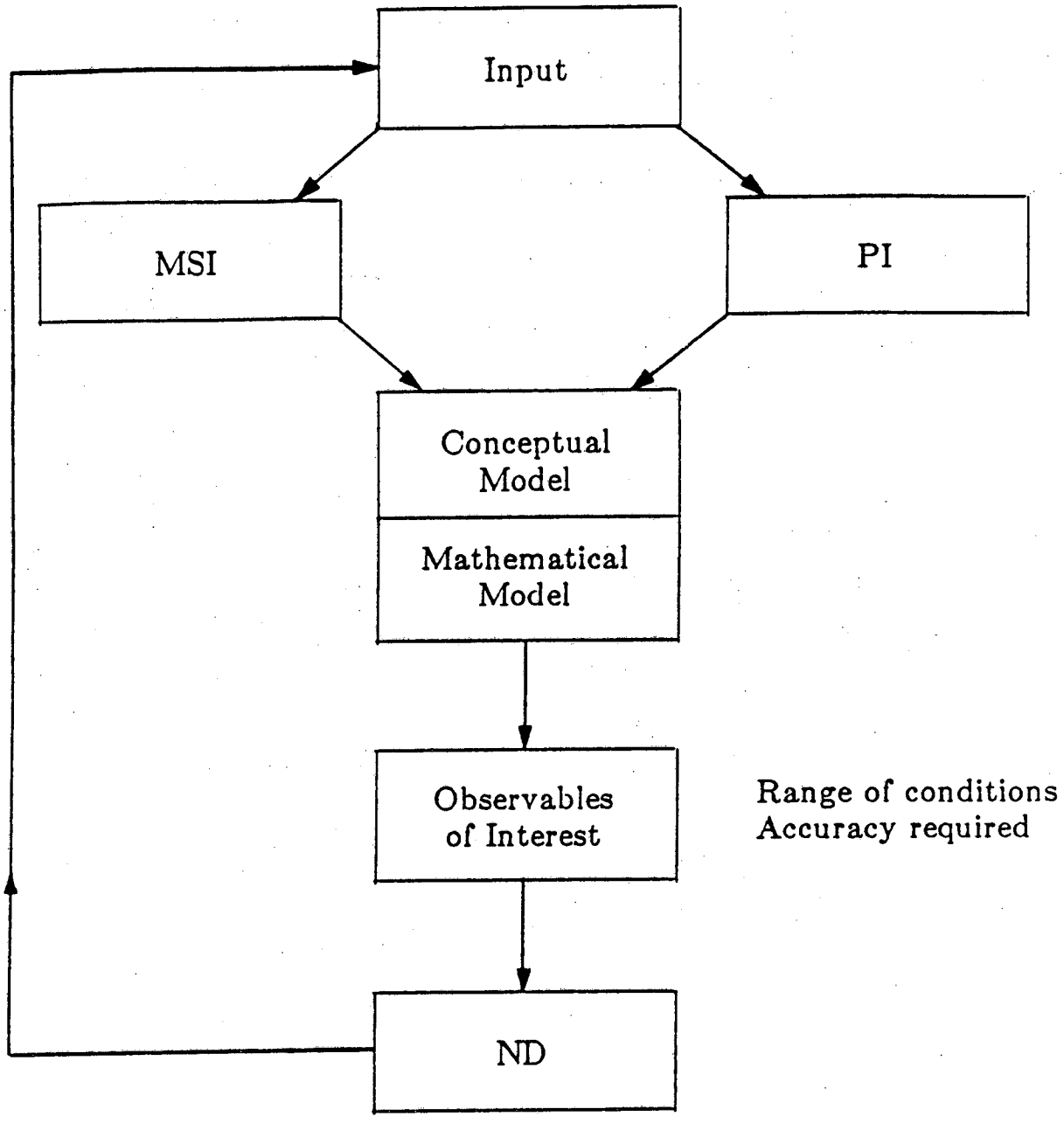

MSI = Model or Geometrical Structure Identification

PI = Process Identification

ND = Network Design for further measurements

Figure 1. A modeling procedure for validation.

Table 1.
Validation: Two Aspects, Two Stages and Three Elements.

Two aspects	(a) Appropriate Processes (b) Model or Geometric Structures (including boundary conditions)
Two stages:	(a) System Comprehensive, or Basic Understanding, or Process and Structure Identification (b) Performance measures; to Simplification or idealization; to Bounding or sample calculations; to Sensitivity and ranges of applicability
Three elements:	(a) Validation of procedures for process and and structure identification (b) Validation of procedures for conceptualization or simplification (c) Validation of predictions of responses of processes and effects of structures

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