THE PERSPECTIVE OF THE WASTE MANAGEMENT RESEARCH PROGRAM AT NRC ON MODELING PHENOMENA RELATED TO THE DISPOSAL OF HIGH-LEVEL RADIOACTIVE WASTE

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ABSTRACT

Modeling the geologic disposal of high-level radioactive waste falls short of ideal for a variety of reasons. The understanding of the physical processes involved may be incomplete or incorrect. It may not be possible to specify mathematically all relationships among the processes involved. The initial conditions or boundary conditions may not be known or directly measurable. Further, often it is impossible to obtain exact solutions to the mathematical relationships that constitute the mathematical model. Finally, many simplifications, approximations, and assumptions will be needed to make the models both understandable and calculationally tractable. Yet, modeling is the only means available by which any quantitative estimation of the expected performance of a geologic repository over the long term can be made. If modeling estimates of the performance of a geologic repository are to provide effective support for an NRC finding of reasonable assurance of no unreasonable risk to the public health and safety, then the strengths and limitations of the modeling process, the models themselves, and the use of the models must be understood and explored fully.

INTRODUCTION

Due to the long isolation times involved in the disposal of high-level radioactive waste (HLW), there is no way that a prototypical geologic repository can be constructed and tested fully over its isolation period to provide a complete set of empirical information on how it will work. Demonstrations of compliance with regulatory criteria will consist of extrapolations of short-term tests to long-term situations. Moreover, since a complete system test is equally impractical, the tests upon which the extrapolations are based will be conducted only for various components of a repository. Various types of models are expected to be used by the United States Department of Energy (DOE) in demonstrating compliance of deep geologic disposal of HLW with the requirements of the U.S. Nuclear Regulatory Commission's (NRC's) Part 60 of Title 10 of the U.S. Code of Federal Regulations[1-4].

DOE will employ various types of mathematical models which represent the processes and phenomena which have to be considered in understanding repository behavior. Due to the complexity of HLW disposal systems, extensive use of simplified models is expected[4]. Part of the demonstration of reasonable assurance that regulatory requirements are satisfied is to show that the models used, simplified or not, are adequate representations of reality. In the case of simplified models, a clear statement of the price of the simplification will be needed, e.g. what phenomena or interactions of phenomena have been left out of the simplified model. A major goal of NRC's program of HLW research is to ascertain the price of simplification of models and to be able to judge what simplifications are acceptable.

DOE bears the responsibility for demonstrating the safety of a HLW repository and thus is responsible for all aspects of development of models, any associated computer programs, and their validation. NRC will review DOE's license application, including supporting technical analyses, and must develop the technical expertise necessary for a licensing review. Also, the Nuclear Waste Policy Act (NWPA) of 1982, NRC's regulations, and an interagency procedural agreement provide for extensive pre-licensing consultation by NRC and DOE on technical issues, including questions about the development of models and any associated computer programs. NRC's HLW research program is aimed at developing essential technical expertise including, in some cases, independent development of models, means of obtaining data for models, and computer programs to support both pre-licensing consultation and licensing reviews.

The remainder of this paper discusses briefly the perspective of NRC's HLW research program on modeling in HLW disposal. Topics covered are the modeling process and its relationship to HLW disposal and the current status of modeling for HLW disposal.

THE MODELING PROCESS

Qualitative and Quantitative Models

In the process of modeling a set of physical phenomena, two kinds of models are considered: qualitative and quantitative. A description of how mathematics is used to model the physical processes relevant to HLW disposal is given in the Appendix. A qualitative model is a verbal description of the physical processes that are taking place. This kind of model is often called a conceptual model. What a modeler considers to be an adequate qualitative model is always a matter of judgment. The accuracy of a qualitative model is a measure of how closely it describes the physical processes under consideration. One always has to formulate a qualitative model before emulating it with a quantitative model. The quantitative model consists of a set of mathematical relationships which are intended to describe in a precise way the interactions among the phenomena that make up the physical processes which are described verbally but imprecisely in the qualitative model. Numerical values of physical quantities (dependent variables) which characterize the consequences of the physical processes can be obtained from quantitative models, but not from the qualitative models.

One should bear in mind that a quantitative model will not be any more accurate in mapping the physical processes being modeled than the qualitative model from which it was derived. For example, if one assumes that the density of water is independent of temperature and incorporates this assumption into a mathematical model of ground water flow in a repository of HLW, then the buoyancy induced flows which will occur if temperatures are high enough will not be predicted by the mathematical model.

Quantitative models are generally formulated under the assumption that one is given a set of well defined parameters in the form of initial conditions, boundary conditions, and properties. In an ideal situation, the following conditions would hold throughout the modeling process. The qualitative model would account for all physical processes and relationships that need to be taken into consideration to describe accurately the situation being examined. The quantitative model would specify accurately all of the precise mathematical relationships needed to emulate the qualitative model completely. The parameters would be known exactly and one would be able to obtain exact values of the desired physical entities, throughout the space and time of interest (the ranges of independent variables), from the mathematical relationships that comprise the quantitative model.

Direct and Inverse Problems

Modeling problems in which the parameters can be specified a priori, as in the ideal situation described in the previous paragraph, are said to be mathematically well posed because there is enough information available to solve them and there is assurance in many situations that the solutions obtained are unique. Such problems are also called direct problems. In HLW disposal applications, what is possible or practical to measure at a prospective site is often an indirect measure the site's properties or boundary conditions. The mathematical problem then becomes "Given that what is measured at the site is functionally related to the physical properties of the site that are the proper conditions for a model, how is this functional relationship derived and how are the measurements to be translated into initial conditions, boundary conditions, and properties?" In mathematics, such problems are known as inverse problems and they are mathematically "ill posed" because there is no assurance that their solutions are unique[5]. There could be many combinations of parameters, i.e. conditions, which could reproduce what is measured at the site. The process of obtaining possible sets of paramters from ill posed problems has been given the name model calibration in HLW and other hydrological applications.

Other Limitations of Modeling

In reality, the modeling process is nearly always less than ideal. Simplifying assumptions and approximations can be and often need to be introduced into every step of the modeling process. Two examples of such simplification in HLW applications are the treatment of systems of fractures as equivalent porous media and the lumping of complex geochemical effects into single distributuion coefficients.

Modeling falls short of ideal for a variety of reasons. The verbal description in the qualitative model may be incomplete or incorrect. It may not be possible to specify all of the mathematical relationships needed for the quantitative model. As indicated in the previous section, the initial conditions, boundary conditions, and properties may not be well known. Finally, even if the quantitative model is completely faithful to the qualitative model, it is very often impossible to obtain exact solutions to the mathematical relationships that constitute the quantitative model.

Solution Procedures

The mathematical relationships that make up the quantitative models in HLW applications are generally continuous in nature in that they describe continuous changes in time and space. Exact solutions of the mathematical relationships would describe continuous temporal and spatial distributions of the physical quantities being sought. When exact solutions can not be obtained, there are many ways in which approximate solutions can be obtained. One particularly attractive avenue to obtaining approximate solutions is to resort to numerical methods by establishing discrete mathematical relationships which are approximations of the quantitative model's continuous relationships. This approximation is accomplished by selecting a finite number of points in space and time and examining how the continuous relationships may be approximated by making use of the values of the desired physical quantities at those points. The solutions obtained from the approximate discrete relationships give values of the desired physical quantities only at the preselected finite number of spatial and temporal points. With a correct approximation procedure, the closer together are the spatial and temporal points, the better the approximation. The discrete relationships are usually cast in such a way that they can be solved algebraically.

The Role of Computers

The numerical solution procedure described above is always mechanical and repetitious, and therefore amenable to digital computer programming. Computer programs, or codes, can be written to implement the desired numerical solution procedure on a high speed digital computer. Alternatively, if exact solutions of the mathematical relationships of the quantitative model are available, computer programs are often written in order to extract numerical values from the expressions making up the exact solutions. The computer program is often the most visible element of the modeling process because the program can be used to obtain numerical values of the desired physical quantities in fairly short order. This aspect of computer programs has led to the unfortunate term "computer model," although computers themselves are totally incapable of performing any part of the task of model formulation. The computer program is merely a set of instructions which a digital computer follows to carry out the numerical solution procedure or to evaluate expressions making up exact solutions. In either case, the use of computers introduces additional approximations and additional elements of judgment into the modeling process. The approximations arise from the fact that computers cannot be infinitely precise in their manipulation of numbers. A poor selection of a numerical method can have disastrous effects on the results obtained from discrete approximation procedures. When computers are used to evaluate expressions for exact solutions, one has to bear in mind that those expressions are often replaced by approximate representations and the numbers obtained from the computer are actually obtained from the approximate representations.

Physical Models: Analogues and the Principle of Similarity

Very often when a model of a physical phenomenon is being formulated, either in the qualitative or quantitative stage, it becomes apparent that the description which is evolving is similar in some way to the description of another, perhaps seemingly unrelated, phenomenon. Such similarities between apparently different phenomena are called analogues. There are well known analogues between electrical systems and mechanical systems and between electrical systems and thermal systems which stimulated the use of analogue computers. One can exploit the analogy between phenomena to perform experiments with one phenomenon to provide information about the other phenomenon or to exploit existing empirically obtained information about one phenomenon to learn about the other phenomenon. Such experiments are conducted or exploited because they are in some sense tractable while experimentation on the phenomenon of direct interest is not. For example, NRC is funding research using natural and man-made analogues to study the properties of "aged" boroslicate glass waste forms.

In addition to laboratory experiments involving analogues, the natural environment provides analogues for understanding different parts of an HLW system. NRC is examining radionuclide behavior around ore bodies as analogues for understanding radionuclide migration from a HLW repository, and geothermal sites provide analogues for understanding the possible couplings of thermal, hydrologic, mechanical, and chemical effects which may occur near emplaced HLW.

There is also another kind of physical model which is based on the principle that experiments on the same phenomenon can be conducted on several different scales (e.g. length and time scales). This principle is known as the principle of similarity and is based on the idea that there are dimensionless parameters (ratios involving physical properties, length scales, and time scales) whose equality between two tests insures that the two tests are similar to each other. These ratios are obtained from the mathematical model and do not require a solution of the relationships which make up the model. Dimensionless parameters are also useful in generalizing the results of mathematical models. A laboratory experiment which is similar in the above sense to the conditions under which one would wish to observe the "real system" but can not, say because of inordinate size or long times required, can provide all the information which is needed about the "real system," provided that the relevant phenomena are fully understood and correctly represented by the mathematical model. NRC is funding research on exploiting the principle of similarity to understand heat transfer from emplaced HLW, flow and transport of water and contaminants in saturated fractured rocks, and of the retardation of radionuclides in packing materials around HLW packages.

Validation of Models

In the absence of any confirmatory experimentation, the formulation of a model is purely a hypothetical exercise. On the other hand, experiments themselves are designed with some sort of model in mind. Experimentation and qualitative and mathematical modeling do form alternative lines of inquiry which can show whether a particular phenomenon is understood well enough that its model is in some sense "valid." For phenomena which are not particularly well understood, an iterative process is necessary in which experiments (possibly involving physical models) and models (possibly involving qualitative, mathematical, and complementary physical models) are designed and tested over and over with successive refinements until there is confidence by both the experimentalists and the modelers that the phenomena are sufficiently well understood that the models which have evolved can be used with confidence to extrapolate the behavior of the phenomena under conditions and over times that can not be observed. This process is called validation.

STATUS OF MODELING FOR DEEP GEOLOGIC DISPOSAL OF HLW

Waste Package

Models, both qualitative and quantitative, for the breachment of the overpack and canister of the waste package after the containment period (300 - 1000 yrs) remain inchohate. Reliable ways to extrapolate expected long-term behavior from better understood short term models do not exist. Moreover, radiation and thermal effects on the degradation of overpacks and canisters are poorly understood for both the short and long terms. Work on corrosion of overpacks perhaps has overemphasized uniform corrosion when pitting corrosion may be a more likely and more catastrophic mode of breachment of HLW packages[6, 7].

Mechanisms of leaching and dissolution of radionuclides from the waste form are somewhat better understood than canister failure. However, some controvesy remains over whether leaching or dissolution is the dominant release mechanism. The problem of modeling the influence of elevated temperature on the release of radionuclides from the waste form still needs to be solved[7].

Flow of Groundwater

The flow of groundwater in saturated media is well understood for porous media but not so well understood for fractured media. There are several qualitative models of isothermal flows in saturated fractured media, in the absence of empirical verification, which seem to be sound. These models include equivalent porous media, dual porosity media or more complex multiple interacting continua, and discrete fractures[8]. Recent field studies funded by NRC indicate that treating fractured media as equivalent porous media may be permissible in some instances[9]. Each of these models forms the descriptive basis for a corresponding quantitative model. Very little field testing of the quantitative models has been done and procedures for using field tests to select appopriate models and obtain parameter data for them are still uncertain. Very little is known quantitatively about how thermal effects on fracture apertures and rock properties will influence groundwater flows in saturated fractured media. Also, very little is known about how geochemical effects such as mineralogical alteration can change the flow paths[10]. For flows in unsaturated media, even the qualitative models are still controversial[6, 11]. In both saturated and unsaturated flows, the specification of boundary conditions remains controversial because of the difficulty of selected the "boundary" of a natural groundwater system.

Transport of Radionuclides

In the deep geologic disposal of HLW, radionuclides are expected to be carried from the emplaced waste to the accessible environment through transport by the groundwater. Heat and possibly salt also can have a major impact on transport of radionuclides. While experts are in general agreement on the qualitative description of transport processes, uncertainty and controversy remain over how quantification should be done. The major sources of uncertainty in transport modeling are hydrodynamic dispersion and geochemical retardation. There are also other presumably secondary sources of uncertainty whose effects are more difficult to identify in field situations. For example, matrix diffusion is often ignored but may be of comparable importance to dispersion and geochemical retardation[12].

Dispersion

Although some controversy remains over whether commonly used Fickian dispersion models are correct, such models are generally accepted as being correct for long times[6, 13]. Most uncertainty related to dispersion arises from the inability to measure accurate dispersion coefficients for use in transport models. Experience with comparing predictions by transport models to observed field data has shown that dispersion coefficients increase with distance from the source of contaminant transport[6, 13]. For applications to HLW disposal, dispersion coefficients are measureable only on a much smaller scale than the one required for HLW transport analysis. Recently a method has been developed for predicting large length scale dispersion coefficients from stastical analyses of locally measured hydraulic conductivities but the method has not been validated in the field[13].

Geochemical Effects

There are several ways in which geochemistry can affect transport of radionuclides. Near the emplaced HLW, eleveated temperatures can cause alteration of minerals, possibly changing flow paths, and change the sorptive characteristics of the rocks through which radionuclides will travel[10]. Radiolysis from the emplaced HLW can alter groundwater chemistry so that the water's ability to contain radionuclides is changed. Radionuclides released from the waste package may have a high enough concentration to alter significantly the density of the water-radionuclide mixture. Farther from the HLW, radionuclides are expected to occur in trace amounts so that the density of the water-radionuclide mixture is essentially that of the water. As radionuclides migrate through the host rock, they may adsorb onto or desorb from the host rock.

In HLW applications, most geochemical modeling to date has been concetrated on the migration of trace amounts of radionuclides through the host rock. For each elemental radionuclide, a transport equation for the radionuclide's concentration is examined. The transport equation is linked to other transport equations because of radioactive decay and production by parent radionuclides. The transport equation is porosity-averaged over a volume of rock and water so that both solid and aqueous concentrations are present in the transport equation and there are twice as many unknowns as equations. A common practice is to halve the number of unknowns by specifying a priori the derivative of the solid concentration with respect to the aqueous concentration. This derivative (a ratio in chemical equibrium situations) is also called a distribution coefficient and is measured in laboratory experiments and used in the transport models[14, 15]. Critics of this approach point out that it omits any explicit consideration, via modeling, of the sorption processes and the laboratory measured distribution coefficients are not applicable to field situations[15]. In addition, Rubin[16] has shown that, at a minimum, one must consider speciation by solving transport equations for the chemical compounds in which the elemental radionuclides occur and one must consider whether the reacting species are in an equilibrium or kinetic situation.

Very little modeling in HLW applications has been done on alteration of flow paths, changes in sorptive characteristics of rocks, changes in groundwater chemistry, or the transport of radionuclides in larger-than-trace quantities. At a June 1984 OECD/NEA workshop on geochemical effects on transport[8], there was general agreement that the modeling approach outlined in the previous paragraph is inadequate. There was also general agreement that an adequate thermodynamic data base needed for a good phenomenological geochemical model does not exist, but there was considerable debate about what constitutes a "good" phenomenological geochemical model.

To date, all of the considerations of geochemical modeling discussed above have been given some thought by various investigators for flows in saturated porous media. While many of the ideas developed may carry over to saturated fractured media, very little research has been done on the effects of geochemical retardation on transport in unsaturated media.

SUMMARY AND CONCLUSIONS

The preceding discussion focused on the current status of modeling the numerous phenomena involved in the geologic disposal of HLW. Clearly, much work, basic scientific work, needs to be done before the controversies, uncertainties, and ignorances are resolved, defined, and removed. Yet licensing decisions will need to be made, and will be made long before this happy state is reached - if ever. Fortunately, complete knowledge, certainty, and total agreement among experts is not needed to make competent and confident regulatory judgments. NRC's regulatory judgments are just that - judgments - albeit founded in and supported by scientific understanding and technical analyses. Hence, clear identification and delineation of areas of controversy, uncertainty, and ignorance are useful and necessary to the regulatory process in dealing with areas where definite experimental observation and demonstration are not possible. This is precisely the thrust and focus of NRC's HLW research program. What has been learned already about what is not understood in dealing with the phenomena involved in geologic disposal of HLW has allowed NRC not only to identify and define technical issues that need resolving and minimize the need for conservatisms, but also to draw upon what is understood to provide guidance to DOE through the ongoing public NRC/DOE dialogue taking place prior to license review. Ultimately, NRC's technical base supported by this research will be used to review DOE's license applications and formulate and apply conservatisms, so that confident licensing assessments can be made.

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APPENDIX
THE CORRESPONDENCE BETWEEN PHYSICS AND MATHEMATICS IN MODELING HLW REPOSITORY PERFORMANCE

Before beginning a discussion of modeling, a statement of underlying assumptions and definitions is in order (a metamodel has to be defined). In this discussion, a model is assumed to be a theoretical projection in detail of a possible system of physical relationships. This theoretical projection is a description or an analogue (something which is comparable in certain parts or in whole to another thing) which is used to help visualize something which cannot be observed directly. The modeling process applied to HLW disposal, as with other applications of modeling to technical problems, is based on the principle that the relevant phenomena (the facts, circumstances, or experiences which are apparent to the senses and can be described or appraised scientifically) can be described verbally and mathematically in such a way that there is an isomorphism between the verbal and mathematical descriptions. The objective of formulating a model is to find a way to predict how certain generally unknown mathematical quantities (dependent variables) vary over given ranges of space and time (quantified by independent variables) based on 1) relationships derived from observation and theory and 2) a given set of constraints which are characterized by parameters (quantities or constants whose values vary with the circumstances of their application).

There are four major categories of phenomena which have to be understood in order to predict the performance of a HLW repository: fluid mechanics, chemistry, heat transfer, and solid mechanics. All of the major dependent variables are expressible as potentials whose spatial variations characterize movement of water, transport of chemical species, heat transfer, and deformation of solid rock. The mathematical expressions which characterize the spatial variations of the potentials, the gradients, characterize the physical movements or deformations mentioned above. Each gradient has a primary movement or deformation associated with it, e.g. temperature gradients cause heat transfer. In a physical system where more than one potential is needed to desribe the system, movements or deformations due to the interactions of the phenomena which occur are also possible, e.g. a temperature gradient could also cause a movement of chemical species[17]. Each potential is intensive in nature, i.e. the potential is independent of the spatial extent of the system with which it is associated. Each potential contributes to the energy content of the system by acting over a change in an associated extensive dependent variable (one which increases with the spatial extent of the system, e.g. volume or mass). By normalizing the extensive parameters of the system with respect to its total mass or total volume, a set of specific intensive variables is obtained. Mathematical relationships which represent conservation of mass, charge, energy, and momentum relate the intensive and specific intensive variables to each other. Equations of state provide additional relationships which describe the thermodynamic state of the system and relate potentials and specific intensive variables to each other. Finally, there are empirical or phenomenological relationships (constitutive equations) which relate the movements or deformations caused by variations in the potentials (intensive variables) to the gradients of the potentials. TABLE I lists the potentials, associated extensive and specific intensive variables, and primary measures of movement or deformation for each of the four categories mentioned at the beginning of this paragraph.

Parameters consist of initial conditions (initial values of the potentials specified over the space being analyzed), boundary conditions (histories of the potentials or their gradients specified over the surface enclosing the space being analyzed for the period being analyzed), and properties (the principal characteristics of the substances occupying the space being analyzed). The properties will control how quickly the processes occur and how the dependent variables will be distributed spatially at any given time.

In modeling a physical system, the space being analyzed is generally occupied by the physical system itself. The physical system may consist of several components which are somehow essentially different from each other. There are many ways to divide a physical system into components, one of the more common being by type of material because different materials will have different properties. Regardless of how components are defined, separate components cannot overlap each other spatially and the total space occupied by all components should be the same as that of the overall physical system. At the interfaces of adjacent components within the physical system, there are interface conditions at which movements or deformations related to the gradients in the potentials have to match, and possibly the potentials themselves also have to match. Unlike boundary conditions, interface conditions can not be specified a priori, but they do have to be taken into account when calculations based on a particular model are made.

TABLE I

Major thermodynamic variables in HLW

Category	Potential	Extensive Variable	Intensive Variable	Primary Measure of Move- or Deformation
Fluid mechanics	Pressure, gravity	Volume	Density	Fluid flow
	Shear stress	Deformation rate	Strain rate	Strain rate
Chemistry	Chemical potential	Mass or mole number	Concentration	Flux of chemical species
Heat transfer	Temperature	Entropy	Specific entropy	Heat flux
Solid mechanics	Stress	Deformation	Strain	Strain