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TREATMENT OF UNCERTAINTIES IN THE PERFORMANCE ASSESSMENT OF
GEOLOGIC HIGH-LEVEL RADIOACTIVE WASTE REPOSITORIES

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ABSTRACT

Federal regulations governing the disposal of high-level radioactive waste in deep, geologic repositories require an assessment of performance over thousands of years. Because of the long regulatory period involved and the complex nature of the events and processes of interest, prediction of the performance of the disposal system will inevitably include uncertainties. These uncertainties come from a variety of sources, some are quantifiable and others are not. This paper discusses these uncertainties and outlines approaches for their treatment. Recommendations for the potential resolution of current limitations in the treatment of uncertainties in performance assessment are made. Some general issues, as well as a suggested approach for

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incorporating expert judgment into quantitative performance assessment analysis, are also discussed.

INTRODUCTION

The U. S. Nuclear Regulatory Commission (NRC) has sponsored programs at Sandia National Laboratories, Albuquerque (SNLA) to develop performance assessment methodologies for geologic high-level radioactive waste (HLW) repositories (Cranwell et al., 1982a; Bonano et al., 1987a). Approaches have been recommended and, in many cases, incorporated into the methodologies to treat and/or reduce as much as possible the effect of uncertainties associated with the prediction of repository performance. The purpose of this paper is to summarize the findings of investigations regarding sources and treatment of uncertainties in HLW disposal conducted in the aforementioned programs. Therefore, some discussions presented here have been excerpted from earlier works performed at SNLA. The authors do not intend for this paper to be considered a literature review in uncertainty analysis.

Federal regulations governing the disposal of HLW geologic repositories require an assessment of their performance over thousands of years (NRC, 1983; EPA, 1985). Because of the long regulatory period and the nature of the events and processes of interest, uncertainties are inevitably introduced in performance assessment analysis. These uncertainties arise from several sources, the most important ones being: (1) uncertainty in the future states of the disposal system over the temporal scales set forth in regulations, (2) uncertainty in the models

used to simulate these future states, and (3) uncertainty in the data and parameters required to exercise these models. Modelling uncertainty includes uncertainty in the formulation of a conceptual model for a given state of conditions, uncertainty in the mathematical description of a given conceptual model, and uncertainty in the implementation of a mathematical model in a computer code.

The effect of uncertainties propagates through the overall performance assessment analysis as shown in fig. 1. Uncertainty is initially introduced when the future states of the disposal system are hypothesized. Available system data used to determine these states are used to formulate a conceptual model. These data may not be sufficient and additional information may be required to develop the conceptual model. Next, a mathematical model of the conceptual model is developed. This mathematical model is solved in a computer code. Uncertainty is introduced at this level because of uncertainty in the theoretical description of the processes being modelled, coding errors, and errors in numerical algorithms used in the computer code, to name a few. Verification and benchmarking exercises may be used to build confidence in the mathematical model(s) and associated computer code(s). System data are typically used to produce a calibrated numerical representation of the conceptual model. When data exist, and if time permits, validation exercises may be conducted to provide further confidence in the ability of the model(s) to adequately describe the disposal system and associated processes. Finally, sensitivity and uncertainty analyses are performed to identify and quantify the contribution of parameter and data uncertainty to the uncertainty in the estimate of the performance

measure. Sensitivity analyses are particularly useful in identifying those parameters and processes that contribute most to uncertainty in the performance measure, and consequently, in directing future research and data collection needs.

SOURCES OF UNCERTAINTY IN SYSTEM PERFORMANCE ASSESSMENT

This section summarizes the major sources of uncertainty and their causes. Approaches currently used to treat and/or reduce uncertainty are discussed in a later section.

Uncertainty in Future States of the Disposal System

To perform an analysis of a HLW repository, it is necessary to determine the various states that the disposal system may experience over the time periods of interest. "Scenario" development is aimed at addressing this issue. As used here, a scenario is a sequence of events and processes, either natural or human induced, that could result in the release of radionuclides from the underground facility, their migration through the geosphere and the biosphere, and their eventual exposure to humans. Sources of uncertainty in scenario development include (a) uncertainty associated with the "completeness" of scenarios, (b) uncertainty associated with the probability of occurrence of a scenario, and (c) uncertainty associated with the estimation of the consequences of scenarios. The latter results in uncertainty in the conceptual model for a scenario, uncertainty in the mathematical models representing

relevant phenomena and associated computer codes, and uncertainty in the data and parameters required by the models and codes.

The "completeness" problem in the scenario selection process refers to the uncertainty that all possible scenarios have been considered. Proof of completeness is not possible in the sense that unequivocally all possible scenarios have been considered. The only avenue is to develop logical procedures for scenario selection and screening and submit these procedures to the scrutiny of the technical community (Cranwell and Helton, 1980, 1981). A methodology for the selection and screening of scenarios is discussed briefly later in this paper.

The nature of the scenarios that must be hypothesized is such that the task of assigning probabilities is quite difficult. Uncertainties associated with probabilities can be grouped into either numerical or relative depending on the approach used to derive the probabilities. When sufficient data are available to calculate the probabilities, the uncertainty can be numerical whereas those probabilities estimated based on expert judgement can have relative uncertainties.

Modelling Uncertainty

As was mentioned earlier, modelling uncertainty includes uncertainty in the formulation of a conceptual model of a disposal system for a given scenario, uncertainty in the mathematical model used to represent the conceptual model, and uncertainty in the implementation

of the mathematical model in a computer code. Each of these sources of modelling uncertainty is discussed below.

Conceptual Model Uncertainty

Given a scenario, the state of the disposal system must be hypothesized. This constitutes the formulation of a conceptual model that describes the physical and/or chemical processes taking place, the variables that relate to these processes including boundary conditions, and the spatial and temporal scales of the assumed processes. Uncertainty is introduced in performance assessment calculations when assumptions are made regarding the behavior of the system. Questions such as whether the system is at steady state, or whether it is a porous medium or a fractured medium arise during the formulation of a conceptual model. Frequently, preconceived notions about the behavior of the system resulting from past experiences with apparently similar systems can lead to serious errors in the conceptual model. This has been particularly true when models for saturated porous media have been extended with only few modifications to saturated fractured media and unsaturated fractured media. These extensions have been based on the assumption that the latter two media behave as a continuum much in the same manner as the former. If this assumption is invalid, performance assessment analyses using extended models in saturated fractured or unsaturated fractured media may not be realistic.

The development of a conceptual model implies simplifying the real system so that it can be represented with a tractable mathematical model

that, in turn, can be solved using available analytical or numerical techniques. In addition, typically the "real" system is poorly described making the development of a conceptual model a formidable task. Both of these factors contribute to the uncertainty in the development of a conceptual model. When more than one conceptual model seems to be consistent with available observations, techniques must be developed to reconcile the results of these multiple models. Then, the issue becomes the assignment of probabilities to each of the possible conceptual models.

Mathematical Model Uncertainty

Once a conceptual model has been formulated, a mathematical representation of the models describing the relevant processes is required in order to predict the performance of the disposal system. Mathematical models are required in many areas such as waste/host rock interactions, ground-water flow and radionuclide transport, surface transport and human uptake, and dosimetry and health effects (Cranwell and Helton, 1980, 1981).

Uncertainty in mathematical models will arise because of the lack of knowledge regarding the important processes and associated couplings, a limited capability to mathematically represent the processes and their couplings, insufficient data to describe the processes acting on the system and the system itself, and the extrapolation of the models to temporal and spatial scales beyond those for which they are tested.

The lack of understanding of processes is a fundamental issue that needs to be addressed because it may lead to the development of incorrect models. For example, the assumption that dispersion of a contaminant can be described using a Fickian model has come under severe criticism. Another example of a modeling approach that has been the subject of controversy is the assumption of linear equilibrium to describe radionuclide retardation. Thus, studies aimed at improving the understanding of fundamental processes are required to reduce uncertainties introduced by the theoretical models.

Computer Code Uncertainty

Sources of uncertainty associated with computer codes include coding errors, computational limitations, and user error. Computational errors can be caused by truncation errors due to finite word lengths. Other potential sources of computational errors are the use of imported numerical algorithms with data beyond the required range for a particular algorithm, and user error. The computer codes typically used in performance assessment are particularly susceptible to the latter because of the complexity required to model the relevant processes in HLW disposal.

Parameter and Data Uncertainty

After appropriate mathematical models have been developed and computer codes have been assembled to implement the solution of these models, the modeler is faced with the problem of obtaining suitable

values for the parameters in the models. The uncertainty associated with the values of parameters comes from several sources including (1) measurement error, (2) paucity of data, (3) misinterpretation of data, (4) spatial variation of parameters, and (5) assumptions regarding the behavior of the system. Furthermore, quantifying these uncertainties in order to quantify the uncertainty in the predictions of the models can be difficult.

Several possible sources of measurement error exist. First, the measuring technique may be either incorrect or misapplied. For example, laboratory tests to determine distribution coefficients describing radionuclide/rock interactions might be conceptually incorrect or not applicable under the conditions of interest. Another example is the use of a two-well test to measure hydraulic parameters for rectilinear flow. The two-well test is a potential-type flow experiment in polar coordinates whereas the model for which the measured parameter is intended is not. The implied assumption in this type of experiment is that the medium is isotropic (i.e., a conceptual model has been assumed a priori). The use of accelerated experiments to measure one or more parameters associated with a given phenomenon without proper treatment of other phenomena that may be taking place simultaneously is another example in which the investigator has assumed beforehand the behavior of the system. In this case, the implied assumption is that the time scales of other phenomena are not important. For small temporal- and spatial-scale experiments to be meaningful they must be dynamically similar to the real system. Finally, measurement errors may have a statistical source. For example, many estimators used for the autocovariance and

cross-covariance of spatially variable parameters may be statistically biased.

Parameter and data uncertainty is also introduced because of the spatial variation of the data. Measurements of data often exhibit significant scatter across a site due to the spatial variability of rock properties such as hydraulic conductivity and thickness of geologic units. These properties typically vary in space even if they are measured without error. Uncertainty is introduced by replacing variable parameters with lumped parameters or by representing a random variation with a deterministic but distributed parameter.

The majority, if not all, of the parameters required in performance assessment models cannot be measured directly. Rather, their values are inferred indirectly from excitation-response data using a particular governing equation. The underlying assumption made is that the assumptions implied by the use of a given equation are valid for the system being characterized. In reality, the investigator is deciding a priori the behavior of the system (another example of implicitly selecting the conceptual model prior to the test). This uncertainty can be attributed to the use of existing mathematical equations for given processes and mechanisms beyond their range of validity. As mentioned above the initial source of this uncertainty is really the conceptual model.

TREATMENT OF UNCERTAINTIES

In this section we discuss approaches available for the treatment and/or reduction of uncertainties in each of the areas identified above. We also suggest possible resolutions of limitations in these approaches, and in the case where procedures do not exist, present ideas about how the problem can be addressed.

Scenario Uncertainty

The treatment of uncertainty in the selection and screening of scenarios can be best addressed with a technically sound methodology for scenario selection and screening such as the one described in Cranwell et al. (1982b). The steps involved are (1) initial identification of a comprehensive set of events and processes believed to be important in performance assessment; (2) classification of the events and processes into categories based on the origin and physical characteristics of these phenomena as well as the effect on the disposal system; (3) initial screening of events and processes using well-established criteria such as physical reasonableness, probability of occurrence, consequence, and regulations; (4) combining events and processes to form scenarios; and (5) screening of the scenarios to arrive at a final set for performance assessment.

The contribution of scenario uncertainty to the total uncertainty in model predictions cannot be expressed quantitatively. At most, one

can simply assert that, based on the current state-of-the-art, the suite of scenarios considered is judged to be acceptably complete and decisions based on overall assessment are adequately justified. There is no known procedure for quantifying the effect that failure to identify a scenario will have on the prediction of a performance measure. In principle, the effect of neglecting a scenario in terms of its low probability can be studied using a trial-and-error procedure. That is, repeating the analysis with the neglected scenario included. However, the fact that a scenario has been neglected because of its low probability may be related to the fact that the detailed modelling of the relevant physical processes is itself uncertain (e.g., glaciation mechanisms and the related physical processes are not well understood), and so the value of such a trial-and-error procedure may be questionable.

The scenario selection and screening methodology described in Cranwell et al., (1982b) has been used to formulate scenarios affecting the performance of a HLW repository in bedded salt (Cranwell et al., 1982a), basalt (Hunter, 1983), and tuff (Guzowski, 1987) formations. More uses of this methodology by the international community should be encouraged in order for it to gain acceptability.

A crucial aspect of this methodology, as well as new methodologies that may become available in the future, is the considerable reliance on expert judgment. Expert judgment is necessitated because of the nature of the problem at hand. All six steps in the methodology described by Cranwell et al. (1982b) require to some degree the use of expert

opinion. This is particularly true in the assignment of probability of occurrence to each scenario. Procedures must be developed to incorporate and synthesize expert opinion and associated uncertainties into the methodology.

When sufficient site-specific data exist and the system is sufficiently understood to support the assignment of probabilities, the uncertainty associated with these can be quantified. Techniques for quantitatively estimating the probability of occurrence of scenarios generally fall in one of three categories:

- **Axiomatic** - the event or process is represented by a probability model; available data are used as input to the model; probabilities are assessed based on the output of the model.
- **Frequentist** - data on the event or process are examined for frequency patterns; probabilities are assessed based on the frequency of the data; experiments may be used to obtain the data.
- **Modelling** - conceptual and mathematical models are developed; repeated simulations of the mathematical model are performed; probabilities are assessed based on the outcome of the simulations.

If on the other hand, data are sparse to nonexistent; probabilities are assessed subjectively based on expert judgment. The task then becomes the combination of the numerical uncertainty obtained from data and the "relative" uncertainty obtained from the expert(s). Hunter and Mann (1987) have conducted a literature review that investigated the procedures used in the past for assigning probabilities and the associated uncertainties for geologic events. This study involved the use of a multidisciplinary group of experts. Future activities in the development of techniques for assigning probabilities should be a follow-up of this study.

The combined objective/subjective approach for assigning probabilities should be implemented in conjunction with existing analytical tools in order to concentrate the efforts on those scenarios that are most critical in the estimation of performance measures. For example, the impact of the probability of scenarios on the imprecision of the estimate of a given performance criterion can be investigated with Monte Carlo simulations using ranges and distributions of probabilities. This study could indicate the most important scenarios in terms of demonstrating compliance with the regulations. This is an example of the use of analytical tools to screen out unimportant issues in order to reduce the uncertainty introduced by the use of experts.

Modelling Uncertainty

Conceptual Model Uncertainty

The conceptual model for a given scenario sets the framework for the use of models, computer codes, and parameters in performance assessment analyses. The uncertainty issues that must be dealt with in terms of the conceptual model relate to assuring that all available information about the site and the scenario is used. This information includes hydrologic, geologic, geochemical, and geophysical data. Typically, these data are massive and, as a result, information that does not seem to fit an overall picture suggested by the majority of the data, or by some preconceived notion, is neglected. Inclusion of previously neglected information may lead to a different conceptual model, or perhaps, to multiple models.

The issue that needs to be addressed then becomes whether all this information can be discerned in a logical manner. One possible approach is to use an expert system that asks a series of logical questions. Some of the logical questions are:

- Do the data suggest a steady-state model?
- Do the data suggest a porous media model?
- Do the hydrologic, geologic, geochemical, and geophysical data all suggest the same type of model?
- If one conceptual model is not consistent with all the available data, how many different conceptual models are possible?

An expert system possibly can discern all this information and produce one or more conceptual models and the corresponding limitations of each model. If more than one conceptual model is possible, the expert system could attempt to assign a relative probability to each model based on the fraction of data supporting the model. This approach is a new idea and no indication is available as to whether or not it will succeed in handling uncertainty in conceptual models. However, it seems to be worth exploring. The suggested approach could be similar to that used in the medical sciences to diagnose a patient's illness. A battery of tests are typically performed on the patient to provide specific pieces of information, which when combined with the symptoms the patient exhibits point out a specific medical condition. The expert system is used to discern and evaluate all the information in a systematic and logical manner. In HLW disposal the "illness" is the conceptual model, the "symptoms" are the response of the geologic setting to specifically designed tests, and the "conditions" are steady-state, transient, fractured media, etc..

Mathematical Model Uncertainty

In order to predict the performance of a nuclear waste disposal facility, relevant processes and events must be described with one or more mathematical equations. Site-specific values for the required parameters are supplied, the equations are solved in a computer code, and estimates of the independent variable(s) are generated. The uncertainty in the mathematical description of a real system can only be addressed through model validation activities. "Validation" refers to

the process of obtaining assurance that a model, as contained in a computer code, is an accurate representation of the processes or system for which it is intended. Ideally, validation consists of a comparison between model predictions and observations of the real system. Unfortunately, the temporal and spatial scales required by the regulations precludes the monitoring of the real system so that validation in the true sense can not be achieved. This is precisely the reason why one must rely on predictive mathematical models to show and assess compliance with regulatory criteria.

Given these constraints, some assurance must still be provided that the models used in performance assessment analyses and the assumptions associated with the development of such models are valid to the extent possible. Accepting that "full" validation can never be achieved, a synthesis of laboratory observations, controlled field studies, natural analogs, and expert judgment can be used to ascertain the validity of the models in terms of proper coupling of simultaneous processes, large temporal and spatial scales, and complexity of the system.

Laboratory experiments when carefully designed and conducted can be useful in model validation. The most crucial condition that must be met by laboratory experiments is dynamic similarity with the real system as was discussed earlier. That is, the values of the dimensionless groups that govern the real system must be retained in the laboratory setup. This is particularly important when simultaneous time-dependent processes take place. Accelerating one of the processes while ignoring the time scale of others may lead to biased and, therefore, erroneous

results. Laboratory experiments should not be expected to emulate the real system in its entirety. Rather, they should be designed to study isolated couplings between important phenomena identified with sensitivity analyses.

The use of natural analogs in model validation activities is important to test the ability of the models to extrapolate in time and space. The time scales associated with natural analogs may not be necessarily of the same order as the time scale of waste disposal processes. However, this should not deter the use of natural analogs as they probably may be the only large scale test for certain transport models. The main drawback of using natural analogs may be establishing the initial conditions of the systems. Natural analogs may also play an important role in testing the couplings of simultaneous processes in the models. For example, geothermal reservoirs can be used to test the coupling between ground-water flow and heat transport models.

Controlled field experiments could be useful particularly with respect to the development of ground-water flow models. They could also be used to calibrate and validate this type of model. Care must be exercised in the calibration/validation activities because at least two independent sets of data are required; one for calibration and one or more for validation. The experimentalist must be extremely careful in obtaining assurance that the data sets are indeed independent.

Close interaction between modelers and experimentalists is an important element in the development and validation of sound

mathematical models. Modelers need to be informed of the meaning of measured values of parameters to be used in their models and the dependency of these values on the experiments. For example, laboratory-measured dispersivities can be several orders of magnitude smaller than field-measured values because the measurement of dispersivity is scale-dependent (Neuman et al., 1987). The models must be governed by parameters that can be directly measured in experiments. If some manipulation of experimental data is required to obtain values for the model parameters, uncertainty is introduced in the exercise and thus defeats the purpose of model validation as a mechanism for reducing uncertainty. Interactions between modelers and experimentalists should be structured in such a fashion that the validation exercise is not biased. Every effort should be made to avoid a situation in which the modelling approach dictates to a large extent the manner in which the experiment is conducted.

Computer Code Uncertainty

Uncertainties are introduced into model predictions by the approach used to solve the equations contained in the mathematical models. Errors exist in the approach to discretize differential equations, evaluation of integrals, truncation of infinite series, etc. In general, uncertainties due to computational errors are considered to be minimal compared to uncertainty from other sources in performance assessment. This is the case because of all potential sources of uncertainty computational errors can be minimized through code verification exercises. "Verification" is the process of obtaining assurance that a

computer code correctly implements the solution of a given mathematical model. Code verification is performed by direct comparison of results from a code with the predictions of other codes for the same problem (benchmarking), or with existing analytical solutions for problems that test salient numerical features of the code.

A practical limitation affecting the treatment of uncertainty associated with computer codes in HLW repository performance assessment is the use of large and complex computer codes in Monte Carlo simulations to generate suitable output distributions of the performance measures. The cost of computer time and the need to use large computer systems to run these codes may force the analyst to further truncate parameter sampling schemes. This can result in either reduced confidence in the results or in the possibility that important combinations of parameters may be overlooked in the analysis.

Software quality assurance (QA) is another mechanism for reducing the uncertainty associated with computer codes. Errors in the output from codes may come from various sources. Some of these are:

- Transcription or coding error (e.g., inserting a "+" sign when the original equation requires a "-").
- Use of wrong data (e.g., using a conductivity value when transmissivity is required).
- Incorrect transfer of data between sections of the code (e.g.,

using the stored inverse of a matrix when the matrix itself is required).

- Use of insufficient precision in the algorithms.
- Use of models beyond their range of validity.

The magnitude of coding errors from these sources cannot be estimated either quantitatively or qualitatively. However, the use of strict software QA procedures can significantly reduce the number and magnitude of such errors. Examples of QA procedures implemented for computer software are Lyon (1981) and Wilkinson and Runkle (1986). The former was developed for the Canadian deep geological disposal analysis program whereas the latter has been implemented by SNLA for computer codes developed for the NRC.

Parameter and Data Uncertainty

Because of the complexity of the systems that need to be modeled and the temporal and spatial scales involved, the analyst often is confronted with the difficulty of deciding the values of parameters needed for the analysis. Many of the parameters needed in the models will not be single-valued. There is likely to be greater uncertainty in obtaining single values for parameters than in defining a distribution of values. Therefore, using single values for parameters in the analysis is not acceptable. Several procedures exist for propagating parameter and data uncertainty to the estimation of performance measures. Some of the

most commonly used techniques are (1) statistical methods (including experimental design procedures or Monte Carlo methods), (2) stochastic models, (3) interpolation techniques such as kriging, and (4) differential analysis techniques. Each of these is discussed below.

Statistical Methods. Statistical methods may be classified into the following two categories:

- Experimental Design or Response Surface Methods
- Sampling or Monte Carlo Methods

Experimental design or response surface methods use an experimental design to select a set of specific values and pairings of the input variables for making multiple runs of the computer code. The method of least squares is used with model input and output to estimate the parameters of a general linear model. The use of response surface methods for performing sensitivity and uncertainty analyses can be found in reports such as Iman and Helton (1985). A general and brief discussion on this method is given below.

The estimated model is known as a fitted response surface, and it is this surface that is used as a replacement for the computer model. Thus, all inferences with respect to uncertainty and sensitivity analyses for the computer model are derived from the fitted one. Two points are worth noting with respect to the fitted model. First, a linear model is usually written with an error term added to represent

stochastic variation. However, the actual models considered in performance assessment generally produce deterministic output, and therefore, differences between the fitted model and the actual one are due to lack of fit rather than to stochastic variation. The second point involves individual input variables used in the fitted model. The actual fitting of such a model usually involves additional variables derived from the original variables, such as squares and cross-products as well as transformations of the original variables.

Fitting of a response surface usually requires that some prescription be used to select specific values of the input variables, and more importantly, to determine the manner in which inputs are paired in each of the computer runs. Experimental designs are commonly used to make the determination. The choice of available designs is large. However, one of the more commonly used designs is based on factorial designs.

Factorial experimental designs are well developed in the statistical literature and extensive discussions with respect to them may be found in textbooks on experimental design (e.g., Box et al., 1978). A factorial design utilizes two or more fixed values (i.e., levels) to represent each variable under consideration. Thus, if there are k input variables and if two levels are used for each variable, 2^k possible combinations of the k variables exist, whereas 3^k combinations are possible with three levels, or in general, n^k combinations are possible with n levels. It is also possible to mix the number of levels

used with each variable such as six variables at two levels paired with two variables at three levels and two variables at four levels. One feature of a factorial design is that all pairwise correlations between inputs are equal to zero (i.e., the input values are orthogonal to one another).

Sampling or Monte Carlo methods are based on treating model input parameters as random variables with assigned probability distributions and appropriate correlations. Specific values for model input parameters are selected using available statistical sampling procedures. The sampling procedure generates a number of input vectors that are combinations of values for all parameters in the models to be used. The models are executed for each of the input vectors resulting in multiple values of the performance measure from which a distribution can be obtained.

A number of sampling techniques exist for generating samples of input parameter values: random sampling, factorial stratified sampling, and Latin hypercube sampling. Several of these methods have been compared by McKay et al. (1979) and Filshtein et al. (1981).

Stochastic Models. One approach to reduce uncertainty in parameters is to reduce the number of effective parameters. Incorporation of spatial correlation information in sampling procedures as discussed above is an example. This information can also be incorporated directly into the model by assuming that the random parameters consist of a mean value and a perturbation about the mean. This modelling approach leads

to the solution of two stochastic equations: one for the mean behavior of the dependent variable and another for the variance about the mean. Models that fit this general description are commonly known as "stochastic" models. Stochastic models have been developed for ground-water flow that predict hydraulic heads and, consequently, flow velocities due to the randomness of hydraulic conductivity or transmissivity in an aquifer (Bakr et al., 1978; Gelhar et al., 1979, Gutjahr et al., 1978, to name a few). Stochastic models for contaminant transport in a one-dimensional flow system have also been developed (Gelhar and Gutjahr, 1982; Gutjahr et al., 1985; Bonano et al., 1987b). The latter are based on the assumption that a second-order stationary random velocity field will lead to a stochastic contaminant concentration. Two stochastic models are discussed below: solution of the ground-water inverse problem using geostatistics with conditional simulation, and a one-dimensional stochastic radionuclide transport model.

The inverse problem in general refers to the estimation of the parameters in a model given a known response as a result of a known excitation. In ground-water modeling, the inverse problem specifically refers to the estimation of transmissivity given the hydraulic heads and boundary conditions (Clifton and Neuman, 1982). The combination of the inverse problem in hydrology with geostatistics emphasizes the importance of the spatial correlation of the parameter field to be estimated (transmissivity) and the hydraulic heads. Thus, the effective number of unknowns is reduced. The estimation of the transmissivity field is also conditioned on observations of both transmissivities and

heads. SNLA is implementing a procedure similar to that of Clifton and Neuman. The difference between the two approaches arises because the latter approach does not include co-kriging of the head and transmissivity fields whereas the former does. The general procedure used in the SNLA approach is described by Kitanides and Vomvoris (1983), and Hoeksema and Kitanides (1984, 1985). A model for the statistical spatial variability of the transmissivity field is proposed. The differential equation describing ground-water flow is used to relate the spatial variability of the hydraulic heads and uncertainty in boundary conditions to that of the transmissivity field. A maximum likelihood procedure is used to estimate the unknown parameters in the proposed transmissivity field model conditioned on the observed values of hydraulic head and transmissivity. The variability of heads and transmissivity are used in a linear estimator (co-kriging) to obtain the actual transmissivity field from observations of head and transmissivity. Co-kriging is also used to estimate the variance of the transmissivity field. The spatial variability of velocity fields are related to the variability of head and transmissivity using Darcy's equation. Conditional simulation is used to generate fields of transmissivity, heads and velocities that reproduce the measured values in all realizations. The velocity fields are estimated from the flow model using the head and transmissivity realizations as input. Using the simulated velocity fields, multiple flow paths from the repository to the accessible environment can be generated and used to construct a cumulative distribution function of ground-water travel time. These flow paths can also be used for radionuclide transport models in order to

propagate the uncertainty in ground-water flow parameters to the prediction of concentrations.

A stochastic one-dimensional contaminant transport model can be used to transmit the uncertainty in ground-water flow to transport calculations. This type of model is useful as long as the assumption that most ground-water flow, and hence radionuclide transport, occurs along simple one-dimensional paths such as a streamtube (Bonano et al., 1987b). Models have been developed for a single species (Gelhar and Gutjahr, 1982; Gutjahr et al., 1985) and a two-member radionuclide chain (Bonano et al., 1987b). The single-species model is based on the convective/dispersion equation

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} - \alpha U \frac{\partial^2 C}{\partial x^2} + \beta C = 0$$

where

$C = C(x,t)$ - concentration at location x and time t ,

$U = U(x)$ - ground-water average pore velocity,

α - local dispersivity (constant)

β - decay rate constant for the given radionuclide.

In the stochastic framework, the average pore velocity $U(x)$ is assumed to be a second-order stationary random process in space. That is, not only is $U(x)$ a random process in x , but it has a continuity in x expressed through its correlation structure or covariance function. This, in turn, implies that the concentration $C(x,t)$ is also a

stochastic process. Thus, in the analysis, $U(x)$ and $C(x,t)$ are separated into a mean value and a zero-mean perturbation; that is,

$$U(x) = \bar{U} + U' \text{ and } C(x,t) = \bar{C} + C'$$

where $\bar{U} = E[U]$, $\bar{C} = E[C]$, $E[U'] = E[C'] = 0$, and $E[Y]$ denotes the expected value of Y . Using this perturbation approach, governing equations are derived for the mean concentration \bar{C} and the variance of the perturbation $\overline{C'^2}$ as a function of x and t that can be solved using conventional mathematical procedures.

Interpolation Techniques. Kriging is a statistical technique that can be used to estimate a surface from spatially distributed data. It was named after D. R. Krige, who first applied some of the concepts underlying this technique to problems of ore content assessment. However, the general formulation of the theory was provided by Matheron (1969, 1970), and a number of applications of the technique have been performed at the Paris School of Mines (Delhomme, 1976; Delfiner, 1976). As developed by Matheron, the theory of kriging considers the observation record as coming from the realization of some random function and seeks to construct linear estimators that have the properties of unbiasedness and minimum variance. That is, estimators that will have a satisfactory average behavior when applied to many realizations of the random function.

Kriging has several advantages over alternative approaches such as least squares, polynomial interpolation, and distance weighting of the data. It restitutes the measured values as estimates at the data points whereas the least squares method does not because it is meant for regression rather than interpolation. Kriging will not produce the contortions that result from attempting to force a polynomial to fit the data and makes a minimum of assumptions for the structure of the field. Finally, kriging also provides an assessment of the accuracy of the estimates.

The problem to be solved using the kriging technique is typically the following: Given the values $Z(x_i)$, $i=1,2,\dots,n$, of a surface $Z(x)$ in the plane at the data points x_i , estimate the value of $Z(x_0)$, say $Z^*(x_0)$, of the surface at the point x_0 . The kriging estimate of Z at x_0 is a linear combination of the surrounding data points in the neighborhood of x_0 :

$$Z^*(x_0) = \sum_i \lambda_i Z(x_i)$$

The weights λ_i are calculated such that $Z^*(x_0)$ is an unbiased estimate of $Z(x_0)$, and the variance

$$E\{Z^*(x_0) - Z(x_0)\}^2$$

is minimized.

The capabilities of these techniques has led some users to believe that they are to be used primarily when data are scarce; this is not true. As with any interpolating technique, estimates obtained with kriging (and co-kriging) are more accurate as the number of available observations increases. Since kriging is based on geostatistics, it could be useful in directing future site characterization activities. Specifically, it can be used to optimize the location of future observations so that these will contribute most towards reducing uncertainty. Kim (1985) discusses the application of this concept at a candidate unsaturated HLW disposal site.

Differential Analysis Techniques. With this approach, a first-order Taylor series expansion for the actual model about a vector of base-case values is used to approximate the model (Iman and Helton, 1985). The Taylor series approximation is the starting point for uncertainty and sensitivity analyses based on differentiation. The first step in such an analysis is generation of the partial derivatives required in the series. If the function is relatively simple, these derivatives may be generated analytically or by simple differencing schemes. However, the function may be too complex to permit such simple approaches and more involved approaches tailored to the particular model under consideration must be used.

Once the desired partial derivatives have been obtained, they can be used in the Taylor series. For uncertainty analysis, the Taylor series approximation can be used in conjunction with Monte Carlo simulations to estimate distribution functions. Further, this

approximation can be used to obtain expected-value and variance estimates. For sensitivity analysis, the coefficients in a Taylor series can be normalized. The values of these normalized coefficients can be used to develop rankings of variable importance.

Differential techniques have been widely used in uncertainty and sensitivity analyses and several introductory treatments are available (Tomovic, 1963; Tomovic and Vukobratovic, 1972; Frank, 1978). Examples of the use of differential analysis techniques include Morisawa and Inoue (1974).

From the discussion above it is clear that techniques for treating parameter and data uncertainty exist. Each technique has its advantages and disadvantages, and no technique is generally considered superior to any other. Rather the adequacy of a given technique is usually determined by the particular application and circumstances under which the technique is used.

The treatment of parameter and data uncertainty requires some information about the values of the parameters themselves. This information is typically in the form of probability distribution functions (pdf's), correlations, and ranges of values. Ideally, this information would be inferred from site-specific data. However, under the best circumstances, such data tend to be scarce. Thus, the need exists to develop procedures for examining data generated from site characterization activities to optimize their use in treating parameter and data uncertainty.

Expert opinion is likely to play a major role in this aspect. Due to the paucity of data, many pdf's, ranges, and correlations between parameters are unlikely to be obtained directly from site-specific data. Yet, sensitivity analyses may indicate that some of this information has a significant impact on the estimate of a given performance criterion. This information must then be obtained from expert opinion. An example is the correlation between porosity and hydraulic conductivity. While this correlation may be quite difficult to measure in geologic media, it is probably counterintuitive to rule it out. If this correlation is neglected in sampling schemes, it may result in combinations of values of conductivity and porosity that are not physically possible.

SENSITIVITY ANALYSIS

One approach for reducing uncertainty in model parameters is the use of sensitivity analysis. Sensitivity analysis generally refers to the means of quantitatively estimating the amount of variation in the output of a model due to a given variation in model parameters. In other words, it is a means of identifying important parameters. Hence sensitivity analyses indirectly also identify important phenomena and scenarios that these parameters characterize.

Sensitivity analyses can be used to direct future research efforts towards the most profitable areas needed in the prediction of performance measures. The results of such research activities can be used to refine models and/or define more realistic ranges of parameter

values and , consequently, improve the reliability of the performance measures.

For computer codes that do not implement a stochastic model of the system, two major approaches exist for performing sensitivity analyses. The first involves the use of statistical sampling of input parameter values commonly followed by regression analysis to identify key parameters (Iman et al., 1978). Statistical methods such as this typically fit a polynomial to describe the relationship between input and output parameters. The second approach, sometimes referred to as the differential or deterministic approach, uses the actual model of the system to define sensitivity coefficients (partial derivatives of output with respect to each input variable) that indicate the relative importance of input parameters on the determination of the output. The sensitivity coefficients are estimated using either a direct method or the adjoint method (Harper, 1983; Cacuci, 1986). Differential analysis is generally more difficult to implement than statistical methods in that it requires knowledge of the actual mathematical relationship between the output and input variables, whereas statistical methods do not. The primary advantage of the differential analysis method is that it supplies information on the importance of all parameters of interest with one run of the computer code. This can result in savings in computer costs as compared to statistical methods for which multiple runs are required. One promising approach that implements the differential analysis method in sensitivity studies with large models and computer codes such as those used in HLW performance assessment is the Gradient-Enhancement Software System (GRESS) (Pin et al., 1986).

This procedure is contained in a FORTRAN compiler and uses computer calculus to add the capability of determining the partial derivatives (sensitivity coefficients) as part of the output of the computer code.

ELICITATION AND USE OF EXPERT OPINION

Expert opinion will likely play an important role in the treatment of uncertainties associated with the performance assessment of HLW repositories. It is customary to think of using expert opinion to treat unquantifiable uncertainties. However, expert opinion will also be important in treating quantifiable uncertainties as well; for example, the assignment of scenario probabilities, and ranges and distribution of parameters.

The type of issues to be addressed by experts will vary dependent on the type of uncertainty in question. For example, the issues associated with parameter and data uncertainty are different from those associated with uncertainty in the conceptual model. Consequently, the approach to elicit and use expert opinion is likely to be unique in each case. However, there are general guidelines for the elicitation and use of expert opinion regardless of the particular situation being addressed. Some of these guidelines are presented below following the review by Mosleh et al. (1987).

Expert opinion can be formulated using a single expert or multiple experts. In both cases, techniques must be developed for improving the estimates provided by the experts. These estimates are biased by

systematic overestimation or underestimation, and overconfidence. Techniques are available for dealing with these biases that could be adopted in HLW performance assessment. One approach is to screen issues prior to presenting them to the expert(s). That is, limit the number of issues that the expert(s) are to address by preliminary elimination of those issues that are not important. For example, in parameter and data uncertainty, sensitivity analyses could identify those parameters and possible correlations that significantly impact the estimate of a performance measure. By screening out unimportant parameters and scenarios, the expert(s) can concentrate on a smaller number of issues and reduce the possibility that their judgment may be affected by unimportant ones. Another approach is to decompose the problem into subproblems that are easier to formulate than the complete and, likely, more complex problem. The expert(s) can be asked to address issues in each part of the problem and the analyst then synthesizes their results. Finally, experts should be encouraged to find evidence that may contradict their views in order to reduce overconfidence.

An important factor in the elicitation and use of expert opinion is whether a single expert or multiple experts need to be used. If a single expert is to be used, then the analyst must carefully select the expert as he will not be contradicted in rendering judgment. If multiple experts are used, techniques must be implemented for the aggregation of their opinions. These techniques are classified into two areas: mathematical methods and behavioral methods for reaching consensus. Mathematical methods are generally preferred but there are situations in which behavioral methods can yield acceptable results.

When using multiple experts several decisions must be made. The analyst must decide whether the group needs to be a multidisciplinary one. This is likely to be the case in HLW performance assessment. In the case of a multidisciplinary group of experts, Mosleh et al. (1987) suggest using multiple groups. Structured interaction within the members of a given group but not among groups is recommended.

Uncertainty analysis in the performance assessment of HLW repositories is a prime candidate for the systematic use of expert opinion. The approach suggested here for the incorporation of expert opinion into the treatment of uncertainty in the performance assessment of HLW repositories is the following:

1. Identification of areas in which expert opinion is needed or recommended in uncertainty analysis.
2. Identification and screening of important issues to be considered by the expert(s) in each of these areas.
3. Compilation of available techniques for the elicitation and use of expert opinion that are appropriate for identified issues.
4. Classification of the issues according to acceptable elicitation techniques that are recommended for each category (e.g., single expert vs. multiple experts).
5. Identification of areas for which decomposition is likely

to be more useful than direct assessment of the complete problem.

6. Elicitation and use of expert opinion to address the issues identified above.

CONCLUSIONS

Uncertainties are introduced at every step in the performance assessment of a HLW repository mined in deep geologic formations. The sources of these uncertainties and approaches currently available for their treatment have been discussed. The concept of propagating these uncertainties to the estimation of performance measures required by existing regulations has been presented (see fig. 1). The impact of these uncertainties on the estimate of performance measures can be quantified in certain cases and not in others. For those uncertainties for which the present state of the art allows quantification (namely, parameter and data uncertainty), a variety of suitable methods is available. However, the implementation of these methods rely on adequate characterization and understanding of the disposal system (e.g., more data for determining probability distributions, correlations, etc.). Currently, the most pressing need is to develop formal and logical approaches for treating uncertainties that can not be quantified with the present state of the art. A good example of such an approach is the scenario selection and screening methodology described by Cranwell et al. (1982b). Similar methodologies must be developed for conceptual models and model validation. Expert judgment is going to play an

important role in uncertainty analysis as applied to the geologic disposal of HLW. Procedures must be developed for incorporating expert opinion into the analysis, and for the reconciliation of potentially conflicting views. Finally, sensitivity analysis is an important aspect of uncertainty analysis because it identifies the most important factors (processes, parameters, scenarios, etc.) affecting the uncertainty in the estimate of performance measures.

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FIGURE CAPTION

Figure 1. Propagation of Uncertainty in Performance Analysis of Geologic High-Level Radioactive Waste Repositories.

