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Uncertainties Associated with Performance Assessment of High-Level Radioactive Waste Repositories

A Summary Report

Prepared by
P. A. Davis, E. J. Bonano, K. K. Wahi, L. L. Price

Sandia National Laboratories
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Prepared by
P. A. Davis, E. J. Bonano, K. K. Wahi*, L. L. Price

Sandia National Laboratories
Albuquerque, NM 87185

Prepared for
Division of High-Level Waste Management
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission
Washington, DC 20555
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*GRAM, Inc.
Albuquerque, NM

ABSTRACT

This report culminates work performed by Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (NRC) under FIN A1165 (Technical Assistance for Performance Assessment) on uncertainties associated with performance assessment of HLW repositories. The purpose of this report is to summarize the work in the topical area of uncertainty conducted under FIN A1165. Many different types of uncertainty can affect the performance of an HLW repository. In a performance assessment, these uncertainties should be identified and considered, and to the extent practicable, should be quantified and reduced. Conventionally, the different types of uncertainty are classified in three major categories: uncertainty in the future state of the disposal system; uncertainty in models needed to simulate the behavior of the disposal system; and uncertainty in data, parameters, and coefficients needed for the analysis of the system. All three major categories of uncertainty are covered in this report. The reader should not rely on this report for an in-depth treatise of these types of uncertainty. Only a short overview is presented with numerous references to SNL reports where different uncertainty topics are discussed in detail; as such, this report is not a stand-alone report. The report can be used by (1) managers to familiarize themselves with the issues regarding uncertainty in HLW repository performance and (2) technical staff as a review of SNL's work for NRC in this area.

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1.0 INTRODUCTION AND BACKGROUND

The Nuclear Regulatory Commission (NRC), under its broad grant of authority under the Atomic Energy Act [1954], is responsible for regulating both the peaceful uses of nuclear energy and the radiological health and safety of the public. With respect to the disposal of high-level nuclear waste (HLW) and spent nuclear fuel, the NRC has promulgated technical criteria under 10 CFR 60 [NRC, 1988]. Additionally, the NRC is the implementing agency for the Environmental Protection Agency's (EPA) radioactive waste standards 40 CFR 191 [EPA, 1985].[1]

The Department of Energy (DOE) is responsible for the design, construction, operation, and decommissioning of a geologic repository for disposal of spent nuclear fuel and HLW. This work includes characterizing the site and demonstrating compliance with the appropriate regulations. To show compliance, the DOE is required to develop and implement a comprehensive site-assessment methodology to prepare a license application to be evaluated by the NRC. To facilitate this evaluation, the NRC is developing a licensing assessment methodology. This methodology is to be applied by the NRC staff in evaluating a DOE license and is not intended to guide the DOE efforts.

The NRC's license assessment methodology will consist of plans and guidelines for reviewing both qualitative and quantitative aspects (i.e., performance assessments) of the DOE license application. Sandia National Laboratories (SNL), which developed performance assessment methodologies for the NRC [Cranwell and others, 1987; Bonano and others, 1989a], has been contracted by the NRC to help develop the post-closure performance assessment aspects of the license assessment methodology. This methodology is based on a combination of tools and techniques that provide for an assessment of the potential consequences of locating a HLW repository in geologic media. An integral part of the methodology and its use is the identification, treatment, and reduction of the uncertainties associated with the performance estimates.

This report represents a culmination of two major tasks in FIN A1165 dealing with uncertainties in performance assessments. These tasks have resulted in several reports on the topical area of uncertainty including: (1) the treatment of data and parameter uncertainty [Zimmerman and others, 1990]; (2) scenario development and screening [Cranwell and others, 1990]; (3) scenario probability estimation [Hunter and Mann, 1989

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[1]The United States Court of Appeals, 1st Circuit, 7/17/87, vacated the EPA HLW standard 40 CFR 191 and remanded the EPA individual protection and ground-water requirements for further consideration. While this action by the court may result in numerical criteria that differ from EPA's original values, the content and form of the requirements are not expected to change. Therefore, the processes and parameters identified in this report are expected to be relevant to any revised EPA standards.

and Apostolakis and others];[2] (4) the use of expert judgment [Bonano and others, 1990]; (5) model validation [Davis and Goodrich];[3] (6) uncertainty analysis of ground-water flow models [Zimmerman and others];[4] and (7) overall compliance with the EPA containment requirement [Bonano and Wahi, 1990]. In this report, the discussions on uncertainty presented in the previous reports are integrated and summarized.

1.1 Definition of Uncertainty

In the context of high-level waste repository performance assessments, two types of uncertainty are discussed: data uncertainty and uncertainty about the nature and behavior of the natural and engineered components of the repository system. With respect to HLW performance assessments, uncertainty in the nature and behavior of the system can be subdivided into uncertainty in models of the system and uncertainty in the future state of the system. Data uncertainty can be defined as the estimated amount by which an observed, measured, or calculated value departs from the true value. Uncertainties arising from instrument accuracy and precision are examples of this type of uncertainty. Generally, the effect this type of uncertainty has on performance assessment results can be quantified. Uncertainty in the nature and behavior of the repository system arises from an incomplete knowledge of the natural and engineered components of the system and their current and future behavior. This type of uncertainty is difficult to quantify. Examples of this type of uncertainty include the uncertainty associated with conceptual models of ground-water flow and radionuclide transport and the uncertainty of future changes to the repository system caused by events such as volcanism or faulting.

1.2 Need for Uncertainty Analyses in Performance Assessment

The EPA has stated that performance assessment is to be used in assessing compliance with their containment requirement in 40 CFR 191.13 [EPA, 1985]. The EPA states that a performance assessment is an analysis that "...estimates the cumulative releases of radionuclides, taking into

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[2] Apostolakis, G. E., R. L. Bras, L. L. Price, J. Valdes, and K. K. Wahi, Techniques for Determining Probabilities of Events and Processes Affecting the Performance of Geologic Repositories: Volume II - Suggested Approaches, NUREG/CR-3964, SAND86-0196, Vol. 2, Sandia National Laboratories, Albuquerque, NM, to be published.

[3] Davis, P. A. and M. T. Goodrich, Technical Basis for Judging the Validity of Models for Performance Assessment of HLW Repositories, NUREG/CR-5537, SAND90-0575, Sandia National Laboratories, Albuquerque, NM, to be published.

[4] Zimmerman, D. A., R. T. Hanson, and P. A. Davis, Comparison of Parameter Estimation and Sensitivity Analysis Techniques for Ground-Water Flow Models and Their Impact on Uncertainty in Model Performance Predictions, NUREG/CR-5522, SAND90-0128, Sandia National Laboratories, Albuquerque, NM, to be published.

account all associated uncertainties." Given the nature of the high-level waste problem (i.e., assuring safety over very long time periods and over large spatial domains), it is evident that the identification, quantification, and reduction of uncertainty will also play a significant role in assessing compliance with all of the other regulatory requirements.

The following sections describe the three major types of uncertainties associated with a performance assessment of a HLW repository: uncertainty in the future state of the system, data and parameter uncertainty, and model uncertainty. Each of these is discussed in terms of the source of uncertainty, the treatment of uncertainty in performance assessments, and the reduction of uncertainty.

2.0 UNCERTAINTY IN THE FUTURE STATE OF THE REPOSITORY SYSTEM

While in reality the repository system (geologic and engineered) will be subject to one temporal evolution of environmental conditions, uncertainty arises from our inability to predict what that future state will be. Therefore, the EPA [1985] requires that all significant processes and events that could affect the ability of a HLW repository to isolate the waste effectively to be considered in a performance assessment analysis. The NRC [1988], by reference to the EPA standard, requires the same consideration except that the NRC uses the phrase, "anticipated processes and events and unanticipated processes and events" in place of EPA's phrase "significant processes and events." In either case, the intent is to assure that the repository system, the combination of the geologic barrier and the engineered system, continues to isolate the waste over periods of time so long that environmental conditions could change significantly from conditions today. Note also that the phrase "processes and events" is somewhat misleading because events of concern for repository performance are in reality the results of processes. For example, the formation of a fault through the repository (an event) is the result of tectonic processes. One possible exception to this is the potential for humans intruding into the repository and releasing the waste to the environment. In this case, one could say, for example, that drilling through the repository is either an event or a process.

2.1 Approaches to Treating Uncertainty in the Future State of the Repository System

Currently, there are two main approaches being advocated for addressing uncertainty in the future state of the repository system. These approaches are distinguished by their focus. That is, one approach, referred to as the environmental simulation approach [Thompson, 1988], focuses mainly on processes while the other, referred to as the scenario analysis approach [Cranwell and others, 1990], focuses mainly on events. Both approaches begin by developing a (or utilizing an existing) list of all processes and events believed to be relevant to the repository system behavior. They then screen these events (for the scenario approach) and processes (for the environmental simulation approach) to eliminate unimportant processes and events where unimportant is defined as physically implausible at a specific site (e.g., excavation of the repository by meteorite impact), inconsequential (i.e., no release of radioactivity), and/or unlikely occurrence.

2.1.1 Environmental Simulation Approach

In the environmental simulation approach the most important processes are coupled together in a computer code that can be exercised to simulate time-dependent occurrences of processes and related events included in the model. Uncertainty in the time and duration of simulated environmental conditions is accounted for in the model by allowing uncertainty in the data and parameters input to the model. Consequence modeling (simulation of the release and movement of radionuclides) is then performed by using the results of the environmental simulation as input for boundary conditions and driving forces. The results of consequence modeling are probabilistic, each being a product of the probability that a given environmental condition will occur at a given time and for a given duration, the probability of the data and parameter set used in consequence modeling, and the consequence results. The key to the validity of the environmental simulation approach is the uncertainty in the environmental model formulation (i.e., assumptions), which is not quantified in this approach. A history of the development and application of this approach may be traced in recent literature [INTERA, 1983; Thompson, 1988; Dames and Moore, 1988; Hodgkinson and Sumerling, 1989].

2.1.2 Scenario Analysis Approach

The scenario analysis approach follows the same basic steps up to the point of simulating the temporal evolution of the system. At this point, instead of simulating the temporal evolution of the repository system, the scenario approach combines events and processes to form scenarios. The scenarios are then screened on the basis of the same three criteria that were used for events and processes. For consequence analysis purposes, each scenario has been assumed to occur immediately after the repository is constructed but the consequence results are weighted according to the probability that the scenario occurs. The conditions of the scenario are used to determine the boundary conditions and driving forces used for consequence analysis. This scenario selection and screening methodology, which is described in Cranwell and others [1990], has been used to develop scenarios for assessing the performance of hypothetical HLW repositories in bedded salt, basalt, and tuff [Cranwell and others, 1987; Hunter, 1983; and Guzowski];[5] the Waste Isolation Pilot Plant [Hunter, 1989]; and has been modified in several national waste disposal programs [e.g., Andersson and Eng., 1989; Stephens and Goodwin, 1989].

The consequence analysis for each scenario is conducted via Monte Carlo simulation to propagate the uncertainty in data and parameters through the suite of models and associated codes that simulate the processes included in the scenario. This approach allows a direct mapping of the uncertainty in the occurrence of the scenarios considered and the uncertainty in the data and parameters to uncertainty in repository performance. Using the probability of occurrence of the scenarios, the probability of each simulation in the Monte Carlo approach, and the associated consequence, the results of the consequence analysis can be cast in a variety of ways (e.g., probability distribution function, cumulative distribution function, etc.) to represent uncertainty in the results.

The key steps in the scenario approach are (1) the estimation of the probability of occurrence for each scenario, and (2) confidence that the initial list of events and processes is comprehensive. The EPA considers it appropriate to use quantitative methods as well as expert judgment in estimating scenario probabilities [EPA, 1985]. The information available

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[5]Guzowski, R. V., Potential Scenarios for Use in Performance Assessment of High-Level Waste Repositories in Unsaturated Tuff, SAND86-7170, NUREG/CR-4770, Sandia National Laboratories, Albuquerque, NM, to be published.

for quantitative estimates of scenario probabilities in this case is from historical records and models of the relevant processes. In fact, these models could be the same ones used in the environmental simulation approach.

Three reports prepared by SNL under this project have addressed the issue of quantification of scenario probabilities [Hunter and Mann, 1989; Apostolakis and others, see footnote 2; and Cranwell and others, 1990]. Two of these reports, Hunter and Mann, and Apostolakis and others, also address the quantification of uncertainties in the scenario probability estimate. Hunter and Mann adopted the premise that most natural events and processes can be sorted into three groups; those for which probabilities can be estimated with high confidence, fairly accurately, and with only limited confidence. Cranwell and others [1990] generated probability estimates for meteorite impacts, volcanic activity, inadvertent intrusions, and faulting and did not specifically address uncertainties in those estimates.

Using the framework of decision theory, Apostolakis and others (see footnote 2) describe the basic formulation required for the quantification of uncertainties in the probability estimates. The approach makes use of Bayesian probability theory and combines historical data and model results with expert judgment in a clear and visible manner. Quantifying these uncertainties, in conjunction with using Bayesian techniques to estimate the probability of scenarios, provides a way to quantify the uncertainty in the estimates of scenario probability. Examples of this approach are provided for tectonics and climatology by Apostolakis and others (see footnote 2).

Finally, Apostolakis and others (see footnote 2) also discuss the unique problem of estimating the probability of humans intruding into the repository and releasing radioactive material to the environment. The problem of human intrusion is unique in that a reliable estimate of the likelihood of drilling into or excavating the wastes requires so many assumptions about the future human population, their technologies, and their behavior as to make any estimate virtually meaningless. In Apostolakis and others (see footnote 2), a discussion on the NRC and EPA guidelines is provided along with a review of published approaches to estimating the probability of human intrusion. In addition, a new approach is provided that involves using historical data (drilling records) to estimate drilling rates for various resources. These drilling rates are then combined with the use of expert judgment to yield a probability of human intrusion. However, Apostolakis and others (see footnote 2) propose that, even with this approach, human intrusion should be considered separately from all other scenarios; that is, not combined into an overall risk curve.

2.2 Comparison of the Environmental Simulation and Scenario Analysis Approaches

There is a perception that the scenario approach does not allow a consideration of issues such as: (1) correlation among events and processes, (2) time-dependent processes, and (3) time of occurrence of events and processes. A mathematical development is presented in Cranwell and others [1990] that provides some insights into how these issues can be incorporated into a scenario approach for a probabilistic assessment of a repository system. Furthermore, this mathematical development supports the assertion that the environmental simulation approach and the scenario approach are really quite similar. A comparison between the two approaches was provided to the NRC in the form of a letter report.[6] This comparison revealed that most of the difficulties and drawbacks attributed to the scenario approach exist in the environmental simulation approach as well. Also, from a mathematical point-of-view, the two approaches are shown to be just different ways of partitioning a risk integral.

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[6] Monthly progress report for FIN A1165 from E. J. Bonano (SNL) to David Tiktinsky (NRC) dated June 15, 1989.

3. DATA, PARAMETER, AND COEFFICIENT UNCERTAINTY

In this report the term data refers to directly measurable quantities whereas parameter refers to a quantity derived from data. For example, data could refer to measurements of water levels in wells and parameters would be the mean and variance of the water levels. Model coefficients such as hydraulic conductivity are also derived from data. Following the above example, measured water levels resulting from a stress to the ground-water flow system are used to infer values of hydraulic conductivity. All three, data, parameters, and coefficients, may be used directly in performance assessments. However, their sources of uncertainties are different; therefore, the treatment of uncertainty for each differs.[7]

3.1 Source of Uncertainty

Data uncertainty results from the limited accuracy and precision of instruments as well as from human error. Misreading of instrument display, improper installation of gauges, and mislabeling of data records are examples of human error. Uncertainty in parameters incorporates data uncertainty and, in addition, can be caused by incomplete or biased data sets. For example, it is difficult to obtain large numbers of geological samples for analysis but large numbers are required to infer parameters such as the mean and the variance of a given measurement. Also, laboratory data on geological materials are often obtained from samples that have an inherent bias in that they tend to represent more competent rock. This is due to sample fabrication problems that make it difficult, if not impossible, to prepare intact samples from naturally weak or flawed portions of the stratigraphy. The uncertainty associated with estimates of model coefficients such as hydraulic conductivity arises from data and parameter uncertainty plus the uncertainty associated with the models used to infer the values of the coefficients. For example, using water-level fluctuations to infer values of hydraulic conductivity requires a model of the hydrologic system. Because this is a modeling uncertainty it is covered in a later section of this report.

3.2 Treatment of Uncertainty

Model results, whether they are for environmental simulation models, data interpretation, or consequence analysis, must reflect the uncertainty associated with data, parameters, and coefficients. All of the methods for propagating data and coefficient uncertainty through models are based on the initial step of defining a probability distribution function (pdf) for each model input (data, parameter, or coefficient). Clearly, these distributions should be derived, if at all possible from the available data, parameters, or coefficients. However, given the paucity of information from a typical repository site, these distributions are often based on heuristic arguments. For example, hydraulic conductivities have been shown to be log-normally distributed in some geologic environments. Therefore, this type of distribution is often used for hydraulic conductivities at sites where insufficient information is available to

[7] When appropriate, the term "variable" is used throughout this report to mean either data, parameter, and/or coefficient.

test what type of distribution the site data follow. In the absence of this type of surrogate information, Harr [1987] provides guidelines for the assignment of pdf's based on the concept of maximum entropy. The importance of these pdf's in uncertainty analysis needs to be emphasized, as the results are highly dependent on the assumed form of the pdf's (i.e., normal, lognormal, uniform, etc.) and their associated parameters (i.e., mean, variance, skewness). Most of the effort, to date, has concentrated on developing techniques for propagating the uncertainty in the input coefficients through the models and to the model predictions, with little effort towards generating reliable distribution functions for input coefficients.

Existing techniques for propagating data, parameter, and coefficient uncertainty through performance assessment models have been reviewed by Zimmerman and others [1990]. Only a cursory discussion, based on their work, is given here; details are found in the original reference.

Uncertainty analysis methods may be categorized as: Monte Carlo simulation, replacement models (response surface techniques), differential techniques (direct, adjoint, and Green's function approach), and geostatistical techniques (stochastic modeling using Monte Carlo simulation and spectral analysis). These techniques ascribe quantitative measures of reliability to model predictions based on uncertainty in model input (data, parameters, and coefficients).

Monte Carlo simulation is a sampling-based approach to uncertainty analysis in which model predictions obtained from simulations can be used to construct unbiased estimates of the means and distribution functions of the dependent variable(s) (i.e., the model output). Sampling methods that are used to obtain the samples for a Monte Carlo simulation vary in their ability to capture the probability behavior of the input parameters. Three commonly used sampling techniques are random sampling, stratified sampling, and Latin Hypercube sampling (LHS) [McKay and others, 1979]. Perhaps the most important feature of the Monte Carlo techniques is that an uncertainty analysis is relatively easy to implement and few simplifying assumptions or constraints need be satisfied to apply the method. The technique can be applied to virtually any set of conditions that existing codes can simulate. No modification of the original computer code is required other than assuring that the desired parameters can be supplied as input and the desired output variables can be recorded (saved) for subsequent analysis. The primary drawback is that pre- and post-processor codes are usually required and the computational expense of making numerous model evaluations can be costly. When random sampling is used, a very large number of samples are required to adequately cover the ranges of all the independent variables. LHS, on the other hand, can provide an adequate range coverage with relatively small sample sizes. However, even with LHS, the number of model runs needed to obtain meaningful results using Monte Carlo simulation can be as much as several hundred or even thousands depending on the number of independent variables. This can make uncertainty analysis costly.

The response surface methodology involves three stages of analysis: (1) development of an experimental design to select specific values of model input, (2) construction of a response surface from the model predictions obtained through the use of the selected model inputs, and (3) the use of the response surface model as a surrogate for the original model in uncertainty analyses. For uncertainty analysis, the replacement model is typically used in a Monte Carlo simulation to estimate the distribution of the dependent variable it represents. Because the response surface is inexpensive to evaluate, large numbers of simulations can be made to obtain representative estimates of the distribution of the dependent variable. However, the estimated distribution function will be no better than the response surface approximation to the original model. In most cases, the construction of the response surface is done with regression techniques based on least-squares procedures. Proper experimental design is essential for building a suitable approximation to the original model. Box and Draper [1987] detail the considerations used in selecting an experimental design for response surface applications.

Uncertainty analysis using differential techniques is usually based on developing a Taylor series approximation of the model considered. Typically, only first-order approximations are used. The fundamental step in a differential analysis is the generation of derivatives of the dependent variables with respect to each independent parameter. This can be simple or very complicated, depending on the model analyzed. Most of the effort in a differential analysis is devoted to the calculation of the derivatives required in the Taylor series expansion. As a result, the literature related to differential analysis tends to be dominated by the development of efficient techniques for the calculation of these derivatives. When the models are simple (i.e., when analytical solutions are available), the partial derivatives can be obtained analytically. Calculation of partial derivatives becomes more challenging as the complexity of a model increases. Three common methods of calculating derivatives in the Taylor series expansions are direct, adjoint, and Green's function techniques. The direct and adjoint approaches can be applied to models with algebraic systems or differential equations. The Green's function approach is applied only to models with differential equations. Once the Taylor series approximation has been developed from the partial derivatives, the variance of the model output (i.e., the uncertainty) is estimated by summing over all variables the product of the squares of the partial derivatives and the variance [Zimmerman and others, 1990; Helton].[8] The Taylor series approximation can also be used as a surrogate model in Monte Carlo simulations to estimate model output distribution functions including the expected value and variance of the output [Iman and Helton, 1985]. Because of the local nature of a Taylor series expansion, differential analysis is typically used to study the effects of perturbations about some fixed parameter value, commonly called the model design point.

The stochastic modeling approach to uncertainty analysis consists of separating the governing equations into an expression for the mean value and an expression for the perturbations about the mean or the variance.

[8]Helton, J. C., Applicability of Uncertainty and Sensitivity Analysis Techniques to Nonlinear Models, Letter Report to U.S. Nuclear Regulatory Commission, FIN A1266, September, 1990.

These expression can then be solved either analytically or numerically to yield a direct estimate of the mean and variance of the dependent variable. Stochastic models have been developed for ground-water flow that predict hydraulic heads and, consequently, flow velocities that result from the randomness of hydraulic conductivity or transmissivity in an aquifer [e.g., Bakr and others, 1978; Gelhar and others, 1979; Gutjahr and others, 1978; Bonano and others, 1989b]. Stochastic models for contaminant transport in a one-dimensional flow system have also been developed [Gelhar and Gutjahr, 1982; Gutjahr and others, 1985; Bonano and others, 1987]. These stochastic models of ground-water flow and transport mentioned above are based on the assumption that the field of interest (hydraulic conductivities or velocities) is a second-order stationary random field or, in other words, that the mean and the variance of the independent parameters are constant in space.

3.3 Reduction of Uncertainty

This section discusses techniques used to reduce uncertainty in data, parameters, and coefficients. In reality, a reduction in the uncertainty in the performance assessment results is the desired outcome. Therefore, the inherent assumption in much of the following discussion is that a reduction in uncertainty in data, parameters, and coefficients will result in a reduction in uncertainty in the performance assessment results.

As stated previously, data uncertainty arises out of lack of precision and/or accuracy in measurements, either instrument related or human induced. A means of reducing data uncertainty is to adhere to adequate quality assurance procedures while collecting the data. Once the data has been collected, as is the usual case in performance assessment, data uncertainty can be quantified and propagated through the appropriate model but cannot be reduced.

In general, there are only two means of reducing the uncertainty in parameters and coefficients: (1) obtain additional data needed to infer values of parameters and coefficients, and/or (2) obtain additional information about the values. The following sections describe each of these approaches.

3.3.1 Obtaining Additional Data

Obtaining additional data will reduce uncertainty in the performance assessment results only if the data has a significant effect on the results. Performance assessment generally involves large numbers of input parameters. However, sometimes only a few parameters are dominant with respect to their importance in model results. In an analogous way, only certain locations may be important for spatially-dependent data. Therefore, every effort should be made to identify the most important parameters, and their locations if necessary, prior to allocating resources for obtaining additional data. Determination of important parameters and important locations is the role of sensitivity analysis. The following sections describe sensitivity analysis techniques in general and the special case of spatially dependent data.

In general, sensitivity analysis techniques can be classified as either statistical or deterministic [Doctor, 1989]. Herein, only an overview of each method is described. For a detailed description of each method see Zimmerman and others [1990].

The statistical approach to sensitivity analysis is based on finding a statistical relation between the model input and the model output. If a Monte Carlo approach has been used for uncertainty analysis, then this step can be accomplished by simply regressing the model input against the model output. Stepwise regression has been proposed for simplifying this procedure [Iman and others, 1978] because only the important variables are kept in the stepwise analysis. Generally, the measure of parameter importance (i.e., the sensitivity coefficient) is obtained by forming a regression of the standardized variables where the standardized variables are obtained by subtracting each sampled variable from its mean and dividing it by its standard deviation. This procedure is also performed on the dependent variable. In this way, the magnitude and variance of values do not interfere with identifying the most important variables. Sometimes it is also useful to transform the sampled values of the variables into the ranks of each sample (i.e., replace the value of each variable with the rank of each value from smallest to largest). This technique is useful when the regression model is nonlinear but monotonically increasing.

The differential analysis technique discussed above under uncertainty analysis was initially developed for sensitivity analysis applications [e.g., Cacuci, 1986; Cruz, 1973; Frank, 1978; Lewins and Becker, 1982; Oblow, 1978; Tomovic, 1963; and Tomovic and Vukobratovic, 1972]. In fact, the main step in differential analysis is the calculation of the derivatives relating a change in model output as a function of model input. Normalizing these derivatives yields sensitivity coefficients. Differential analysis is based on developing a Taylor-series approximation for the model considered. Because of the local nature of a Taylor-series expansion, differential analysis is typically used to study the effects of small perturbations about some fixed base-case or design-point value(s). Techniques used to calculate derivatives include direct, adjoint, Green's function, and computer-based methods such as GRESS [Pin and others, 1986]. The choice of a particular technique depends on several factors such as the number of input parameters, the number of output variables (or performance measures), the availability of "off-the-shelf" models or algorithms, and the relative cost of human and computer resources of that technique as applied to the model of interest.

3.3.2 Obtaining Additional Information About the Parameters and Coefficients

Another technique to reduce uncertainty is to obtain or infer more information about the existing values. In general, there are three types of additional information that can be used to reduce uncertainty in parameters and coefficients: (1) "soft data"; (2) correlation between variables; and (3) autocorrelation.

"Soft data" refers to indirect evidence of the value of a given variable. Take, for example, the problem of estimating the porosity of a given geologic unit. In the extreme case, no measurement of porosity may be available. In this instance, we still have information that bounds the value of porosity. That is, we know the value is between 0 and 1 by definition. In another case we may know that, for a given type of media, porosity ranges from 0.1 to 0.3 and, in other cases, we may know that the porosity is always less than a certain value. All of these are examples of the use of "soft data."

Another type of information about existing parameters and coefficients is correlation, either correlation between different variables or autocorrelation. In performance assessment of HLW repositories several variables are expected to be correlated. For example, some investigators believe that porosity and hydraulic conductivity are correlated, with large values of porosity being correlated with large values of hydraulic conductivity. If this correlation was enforced in uncertainty analysis, then the variance in model output would be reduced because it would not reflect combinations of small porosity and large hydraulic conductivity or vice versa. The technique for finding correlation among variables is typically referred to as multivariate analysis. Examples of multivariate methods are multiple regression, discriminant functions, and cluster analysis. Davis [1986] provides a comprehensive discussion on multivariate analysis.

Autocorrelation refers to self-similarities within a set of values of a given variable. This correlation could be either in a temporal or a spatial sense. For HLW performance assessment we are mainly interested in spatial correlation of geologic or geohydrologic variables. This type of autocorrelation analysis is generally referred to as geostatistics. Geostatistics has its origins in the field of mining [Journel and Huijbregts, 1978] and consists of two basic steps: (1) obtaining a model of the spatial variability for the variable of interest; and (2) estimation of the value of this variable at locations other than the observation points. The estimation of the value of the variable includes both the mean value and the variance about the mean. Several approaches are available for obtaining a model of spatial variable [Journel and Huijbregts, 1978 and Davis, 1986]. Most of these approaches require at least local second-order stationarity (i.e., constant mean and variance). Once a model of spatial correlation has been obtained, the most often used technique of estimating or interpolating values of a given variable is kriging. Kriging 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 [1970], the theory of kriging considers the observation record as coming from the realization of some random function and seeks to construct an unbiased linear estimator of the function such that the estimation errors are minimized. The object, then, is to construct an estimator that will exhibit satisfactory average behavior when applied to other 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 observation points and it provides a measure of the estimation error. In theory, this estimation error could be used to identify areas in which additional measurements are needed and, thus, to reduce uncertainty. However, no direct correlation may exist between the kriging error or uncertainty and the uncertainty in the results of performance assessments. For example, a map of kriging errors of hydraulic conductivities may lead one to perform hydraulic conductivity tests in regions that are not along the flow path from the repository to the accessible environment. To utilize geostatistics effectively in reducing uncertainty in performance assessment results requires the development of formalized sensitivity analysis with geostatistical techniques.

4. MODEL UNCERTAINTY

Models, by definition, are simplifications of reality; therein lies their inherent uncertainty. In HLW, both conceptual and mathematical models are used. Simplifications in these models generally take the form of assumptions about such things as the behavior of the system or the accuracy of a mathematical approximation. Because these models are commonly implemented in computer codes, the uncertainty associated with codes is also addressed in this section.

4.1 Conceptual Model Uncertainty

A conceptual model describes the assumed physical and/or chemical processes taking place in the system, the variables and parameters chosen to represent these processes including boundary conditions, and the spatial and temporal scales of the assumed processes. The development of a conceptual model generally involves simplifying the real system for two reasons: (1) selecting a given portion of the entire system needed for the analysis being performed and/or (2) representing the system with a tractable mathematical model that, in turn, can be solved using available analytical and/or numerical techniques. Simplifications are made about the geometry, initial and boundary conditions, material properties, and nature of processes. In addition, the "real" system is often poorly characterized making the development of a conceptual model a formidable task. Both of these factors contribute to the uncertainty in conceptual models.

Currently, there is no methodology that is designed to quantify the uncertainty in conceptual models. Until now, conceptual models have generally been developed based on a "single" interpretation of existing data using expert judgment. A methodology is needed that would force the analyst to examine all available information in a formalized manner thus minimizing biases and arbitrary rejection of data. This methodology could be based on the judgment of multiple experts well-versed in the construction of models for important processes such as ground-water flow and transport. The methodology could allow for the articulation of all the assumptions invoked by these experts and for consistency checks on these assumptions with available data. The methodology could also have provisions for alternative conceptualizations consistent with the data. Finally, bounding analyses and experimental investigations could be included that are aimed at distinguishing between alternative conceptual models and narrowing the options. Bayesian analysis could be used to estimate the likelihood of the fitness of a given conceptual model relative to others.

4.2 Mathematical Model Uncertainty

Once a conceptual model has been formulated, a mathematical representation of the model(s) describing the subsystems and attendant 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, radionuclide transport, human uptake, and dosimetry and health effects [Cranwell and Helton, 1981a, 1981b].

Uncertainty in mathematical models arises from approximations to represent the physicochemical processes with tractable mathematical equations that allow arriving at a solution of the equations. Application of the mathematical models requires a solution of algebraic, differential, and/or integral equations in the models. The solution of these equations can be classified into three major categories: (1) analytical solutions, (2) semianalytical solutions, and (3) numerical solutions. Bear in mind that model equations are often too complicated to have an analytical, or even a semianalytic solution, and the only option in such cases is to solve them by numerical techniques implemented in computer codes. Uncertainty could be introduced in obtaining each of these types of solutions. For example, analytical solutions typically involve functions (e.g., trigonometric functions, Bessel functions, exponentials) which are approximated with a finite number of terms of some infinite series. Uncertainty could be introduced because of truncation of these series or machine round-off. Uncertainty can be introduced in numerical solutions when the equations are discretized. For example, there are differences between the differential equations in a mathematical model and their numerical representation in a computer code with finite differences. Furthermore, numerical solutions introduce additional uncertainties as a result of the discretization of the domain of interest into cells or finite elements. Semianalytical solutions can suffer from the difficulties of both analytic and numerical solutions. Uncertainty in mathematical models is rarely, if ever, quantified in performance assessments. Instead, it is thought to be miminized to an acceptable level by the uncertainty reduction techniques discussed in the following sections of this report.

Sources of uncertainty associated with computer codes include coding errors, computational limitations, and user errors. Like mathematical model uncertainty, computer code uncertainty is rarely quantified in performance assessment. Instead, quality assurance procedures are used to minimize this type of uncertainty.

4.3 Reduction of Model Uncertainty

In practice, the reduction of model uncertainty occurs at the stage that the conceptual and mathematical models have been implemented in a computer code. All of the activities that reduce uncertainty are included in generally accepted computer code quality assurance requirements. The first such activity applies only to the computer code itself. These include all of the quality assurance procedures that should be followed prior to and throughout the development of the code, and also include code maintenance and configuration management procedures once the code has been developed. Examples of code maintenance and configuration management procedures implemented for computer software include Lyon [1981], Wilkinson and Runkle [1986], Silling [1983], and Harlan and Wilkinson [1988].

The next quality assurance activity to be discussed is designed to test the accuracy of the mathematical model as implemented in the computer code. This activity is called verification, which refers to the process of obtaining assurance that a given computer code correctly implements the solution of its parent mathematical model. Verification involves the comparison of the code solution to the analytical solution of the same problem. Another form of code quality assurance sometimes mistakenly thought of as verification is known as benchmarking. Benchmarking is performed when analytical solutions to problems of interest do not exist. It involves performing the same calculation (model simulation) using different computer codes and comparing the prediction of those codes.

The most important method of reducing model uncertainty is validation, which is the process by which assurance is obtained that conceptual and mathematical models, as embodied in a computer code, are an accurate representation of the process or the system for which the models are intended [NRC, 1984]. Thus validation represents an overall test of model uncertainty, including the conceptual model, the mathematical model, and the computer code. In practice, validation exercises test the data input as well as the models [Davis and Goodrich, see footnote 3]. Ideally, validation consists of a comparison between model predictions and observations of the real system over temporal and spatial scales that are relevant to HLW repository performance. However, the nature of the problem (spatial scales of kilometers and temporal scales of thousands of years) preclude such tests. In fact, Davis and Goodrich (see footnote 3) argue that one can never say for sure that a HLW performance assessment model is "valid"; only that it is either "invalid" or "not valid." Despite these difficulties, some confidence must be developed that the models used to represent the real system, and the assumptions associated with the development of such models, are adequate for their intended use (i.e., to assess compliance with specific numerical criteria in the regulations). Davis and Goodrich (see footnote 3) also propose a validation strategy that includes "generic" validation experiments as well as site-specific experiments. Both types of experiments could, in general, include laboratory tests, field tests, and natural analogs.

When carefully designed and conducted, laboratory experiments can be very useful in testing the model validity. Neither laboratory experiments nor the model being validated should not be expected to emulate the real system in its entirety. Rather, they should be designed to study, in a controlled manner, the critical processes or interactions (e.g., isolated couplings between important phenomena) identified with sensitivity analyses. The most crucial condition that must be met by laboratory experiments is their dynamic similarity to the real system. That is, the values of the dimensionless groups (e.g., Reynold's Number) that apparently govern the real system must be retained in the design of laboratory experiments and associated parameters. 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.

Field experiments have advantages over laboratory experiments in that they are performed on a larger scale, both temporal and spatial, and are performed on virtually undisturbed material. These advantages are gained at the expense of a loss of control on boundary conditions and an increase in uncertainty because of the inability to measure all model input and output at all locations.

Natural analogs are phenomena that have occurred in nature over thousands of years and, sometimes, many kilometers. Migration of uranium from an ore body is one such example. The use of natural analogs in model validation activities is important because it tests the ability of the performance assessment models to extrapolate in time and space. The main drawbacks of using natural analogs are the uncertainties in establishing the initial conditions and time history of the system. Natural analogs may also play an important role in testing coupled models that represent important couplings such as between ground-water flow and heat transfer, and between ground-water flow and mass transport. For example, geothermal reservoirs can be used to test the coupling between ground-water flow and heat transfer models.

5. SUMMARY AND CONCLUSIONS

Many different types of uncertainties are associated with the assessment of the performance of a high-level radioactive waste repository. These uncertainties must be identified and should be quantified and reduced wherever possible. Three major categories of uncertainty are (1) uncertainty in the future state of the disposal system; (2) uncertainty in models that are used to analyze repository behavior; and (3) uncertainty in data, parameters, and coefficients used in the analysis of future states of the system and in models of system performance.

Uncertainty in the future state of the repository system is caused by a lack of knowledge of the rates and types of processes that could affect the integrity of the system (e.g., volcanism, tectonics) over thousands of years. This type of uncertainty is generally treated by postulating all possible disruptive events and processes (i.e., scenarios), then screening out those that are highly unlikely to occur at the site. The remaining scenarios are then analyzed by assuming that a given scenario occurs (e.g., a volcanic eruption), analyzing the consequences of such an event, and combining the consequence with an estimate of the likelihood of the scenario occurring to arrive at an overall risk of the scenario. Finally, the consequences from all of the scenarios are combined to form a total estimate of the repository system performance. In this entire analysis it is assumed that the likelihood (or conversely, the uncertainty) of the occurrence of a scenario can be estimated from a combination of historical data, models of the processes which cause the scenario to occur, and expert judgment. An alternative approach is to scenario analysis is to attempt to model the temporal evolution of the repository system. This approach, referred to as the environmental simulation approach, is then combined with consequence models to produce an overall estimate of the repository performance.

Models that simulate the behavior of the repository system for any given scenario can be thought of as a combination of conceptual and mathematical models implemented in computer codes. Models, by definition, are simplifications of real systems; therein lies the uncertainty associated with models. Assumptions made about the real system allow these simplifications to be made. Uncertainty associated with models is rarely addressed directly in performance assessment modeling. However, this type of uncertainty could be quantified by proposing and using multiple equally-plausible models throughout the entire performance assessment. Conceptual model uncertainty can be reduced by validation, and verification can be used to reduce mathematical uncertainty. Uncertainty in computer codes is addressed by adhering to adequate quality assurance programs throughout the life-cycle of the computer code.

Data uncertainty arises mainly from instrument accuracy and precision and from the potential for human error. Parameters, which are derived from data, inherently have the same error as data plus errors of interpretation. Coefficients are values derived from data through the use of a model of the system or subsystem. Uncertainty in data, parameters, and coefficients can be caused by the limited amount (both in space and time) of each available for a given repository system. Performance assessment propagates quantifiable uncertainties in data, parameters, and coefficients through the models that simulate the consequences of waste disposal and results in a distribution of possible outcomes. Uncertainties associated with data, parameters, and coefficients that are difficult to quantify (i.e., human error and interpretation error) are treated through strict quality assurance requirements on data collection and analysis. Uncertainty arising from sparse data and/or parameters is generally treated by assumptions of spatial continuity or correlation. Because this type of uncertainty is based on assumptions, it is a conceptual model uncertainty and should be treated as such. Reduction of data, parameter, and coefficient uncertainty can be accomplished either by gathering more data (i.e., additional site characterization) or by obtaining additional information about the existing data. This information could be in the form of correlations between or among data or by the inclusion of additional "soft" data that constrains the values that the data can take.

Throughout the identification, treatment, and reduction of uncertainty expert judgment will be employed. The only question to be addressed is when and how this judgment will be obtained and documented. Certainly, the use of expert judgment to obtain probabilities of the occurrence of future events or to define ranges of parameter values to use in consequence analysis should be formalized.

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Nevada Operations Office
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Las Vegas, NV 89193-8518

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Regulatory Analysis
Attn: B. Sagar
W. Patrick
6220 Culebra Road
P. O. Drawer 28510
San Antonio, TX 78284

A. L. Gutjahr
Department of Mathematics
New Mexico Institute of Mining and Technology
Socorro, NM 87801

G. Apostolakis
University of California
5532 Boelter Hall
Los Angeles, CA 90024

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Attn: K. K. Wahi
D. A. Zimmerman
R. Knowlton
M. T. Goodrich
C. D. Updegraff
1709 Moon N.E.
Albuquerque, NM 87112

G. de Marsily
Ecole des mines de Paris
35, Rue Saint-Honore
77305 Fontainbleau
FRANCE

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R. L. Bras
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Cambridge, MA 02139

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NAGRA
Parkstrasse 23
CH-5401
Baden, SWITZERLAND

P. Prado-Herrero
CIEMAT
Centro de Investigaciones Energeticas Medioambientales y Tecnologicas
Avda. Complutense, 22
28040 Madrid, SPAIN

A. Nies
Institut fur Tieflagerung
Theodor-Heuss-Strasse 4
D-3300 Braunschweig
FEDERAL REPUBLIC OF GERMANY

B.G.J. Thompson
HM Inspectorate of Pollution
Romney House
43 Marsham Street
London SW1P 3PY
UNITED KINGDOM

T. Vieno
Technical Research Center of Finland
P. O. Box 169
SF-00181 Helsinki 18
FINLAND

Applied Physics, Inc. (2)
Attn: C. L. Lee
J. D. Johnson
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3100 Port of Benton
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Applied Research Technical Services, Inc.
Attn: K. N. Gaither
300 San Mateo Blvd., N.E.
Suite A-220
Albuquerque, NM 87110

Nuclear Energy Agency (2)
Organization for Economic Cooperation and Development
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C. Thegerstrom
38, Boulevard Suchet
F-75016 Paris, FRANCE

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Department Head, Nuclear Fuel Cycle Safety
Ministere de I'Industrie
99, Rue de Grenelle
75700 Paris, FRANCE

A. Alonso-Santos
Universidad Politecnica de Madrid
J. Gutierrez Abascal, 2
28008 Madrid, SPAIN

P. Carboneras-Martinez
ENRESA
Calle Emilio Vargas, 7
28043 Madrid, SPAIN

Sandia National Laboratories

3141	S. A. Landenberger (5)
3151	W. I. Klein
3223	P. A. Davis (5)
6310	T. E. Blejwas, Actg.
6310A	F. W. Bingham
6312	P. G. Kaplan
6313	R. W. Barnard
6317	S. Sinnock
6340	W. D. Weart
6342	D. R. Anderson
6342	M. G. Marietta
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6400	D. J. McCloskey
6410	D. A. Dahlgren
6412	A. L. Camp
6413	F. T. Harper
6413	J. C. Helton
6415	R. M. Cranwell
6415	J. E. Campbell
6415	M. S. Tierney
6416	E. J. Bonano (9)
6416	M.S.Y. Chu
6416	C. P. Harlan
6416	L. L. Price
6416	D. P. Gallegos
6416	N. E. Olague
6416	S. H. Conrad
6416	J. T. McCord
6416	E. R. Lindgren
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6416	P. I. Pohl
6418	S. L. Thompson
6419	M. P. Bohn
8524	J. A. Wackerly

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P. A. Davis, E. J. Bonano, K. K. Wahi[1], L. L. Price

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Sandia National Laboratories
Albuquerque, NM 87185

[1]GRAM, Inc.
Albuquerque, NM 87112

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11. ABSTRACT (200 words or less)

This report culminates work performed by Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (NRC) under FIN A1165 (Technical Assistance for Performance Assessment) on uncertainties associated with performance assessment of HLW repositories. The purpose of this report is to summarize the work in the topical area of uncertainty conducted in Tasks 2 and 3 of FIN A1165. Many different types of uncertainty can affect the performance of an HLW repository. In a performance assessment, these uncertainties should be identified and considered, and to the extent practicable, should be quantified and reduced. Conventionally, the different types of uncertainty are classified in three major categories: uncertainty in the future state of the disposal system; uncertainty in models needed to simulate the behavior of the disposal system; and uncertainty in data, parameters, and coefficients needed for the analysis of the system. All three major categories of uncertainty are covered in this report. The reader should not rely on this report for an in-depth treatise of these types of uncertainty. Only a short overview is presented with numerous references to SNL reports where different uncertainty topics are discussed in detail; as such, this report is not a stand-alone report. The report can be used by (1) managers to familiarize themselves with the issues regarding uncertainty in HLW repository performance and (2) technical staff as a review of SNL's work for NRC in this area.

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