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DISRUPTIVE EVENT UNCERTAINTIES IN A
PERTURBATION APPROACH TO NUCLEAR
WASTE REPOSITORY RISK ANALYSIS

T. F. Harvey

MASTER

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PROLOGUE

Decisions about how to make nuclear waste disposal systems safe for thousands of years require the participation of scientists, engineers, and laymen. Many meetings and conversations with people from different backgrounds have shown the need to bridge the gap between technology and public concern.

The present work describes the major features of a unified probabilistic model for predicting the safety of a waste disposal system. If adopted, such a model could be used to guide national agencies and others in developing a data base required to prove the safety of a disposal plan.

The model itself is not devoid of controversial issues. Nonetheless, it does provide a framework for helping to resolve many of the important issues in the development of a technological data base.

ABSTRACT

A methodology is developed for incorporating a full range of the principal forecasting uncertainties into a risk analysis of a nuclear waste repository. The result of this methodology is a set of risk curves similar to those used by Rasmussen in WASH-1400.⁽¹⁾ The set of curves is partially derived from a perturbation approach to analyze potential disruptive event sequences. Such a scheme could be useful in truncating the number of disruptive event scenarios and providing guidance to those establishing data-base development priorities.

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1.0 INTRODUCTION

In evaluating the hazards associated with the disposal of high-level radioactive wastes in deep geologic strata, we must recognize that uncertainties are implicit in our predictions. These uncertainties do not invalidate the findings of waste disposal studies, but only by properly accounting for the uncertainties can we ensure that conclusions and forecasts can stand up to criticism. Further, it is necessary to quantify the uncertainties to determine which disposal sites are safe and have the greatest margins of safety. By identifying the sources of the uncertainties, we can distinguish between disposal sites that are unacceptable today (but that might become acceptable as technology improves and uncertainties diminish) and those that are clearly inappropriate for waste disposal.

Prediction uncertainties can usefully be separated into four sources:

- Descriptive uncertainties. These include uncertainties in all descriptors (parameters used to describe the disposal site). These include the dimensions of aquifers, porosity of surrounding rock, thickness of rock layers, and temperature.
- Dynamic uncertainties. These are uncertainties in the mathematical model used to predict the future dispersion of the waste. They include uncertainties in such factors as the empirically derived laws that govern the interactions between the waste and the geologic environments.
- Disruptive-event uncertainties. Events such as meteor strikes and earthquakes cannot be predicted, but they can be dealt with statistically.
- Tail-extrapolation uncertainties. Typical probabilistic risk curves have tails that have very low probabilities. Complex systems do not allow sampling of their very low-probability statistical tails. Extrapolation can be undertaken by using curve-fitting techniques. This introduces a curve-fitting uncertainty that can be folded into a probabilistic risk analysis.

If we were to take each of these sources of uncertainty to be independent, the total uncertainty in the predicted hazard from the buried waste could be written as

$$\sigma_{TOT} = \sqrt{\sigma_D^2 + \sigma_P^2 + \sigma_E^2 + \sigma_T^2} \quad (1)$$

where σ_D , σ_P , σ_E , and σ_T represent the uncertainties in the hazard, caused respectively by descriptive, dynamic (predictive model), disruptive-event, and tail-extrapolation uncertainties. The total uncertainty is a reflection of the state of current technology - which determines how accurately we can describe the site and how accurately we can model future behavior - and is a measure of how confidently decisions and predictions can be made. One of the obvious aims of uncertainty analysis is to suggest ways to reduce the size of σ_{TOT} by determining the sources of uncertainty most likely to yield to further work.

1.1 PROBABILISTIC SAFETY GOAL

A decision on the safety of a nuclear waste disposal system depends on a prediction of the performance of the system and criteria against which to judge the predicted performance. When scientific uncertainties are involved in the analysis, a range of values for the performance is obtained which describes a repository's performance. To compare such probabilistic predictions with social values requires a probabilistic performance objective (safety goal).

Besides various daily risks, Fig. 1 shows one such probabilistic safety goal. It starts at a frequency (events/year) of approximately 10^{-2} which corresponds with 10 early fatalities and ends at about 10^{-7} events/year which exceed 20,000 early fatalities. Nuclear accidents producing greater than 20,000 fatalities would thus be expected to produce about 10^{-3} early fatalities/year on the average. This is about three orders of magnitude below the expected fatalities from dam failures, for example.

A probabilistic safety goal like this one can be used to show that repository performance is adequate, resulting in a curve like the dashed "early and latent fatalities" curve shown in Fig. 1. If the "early and latent fatalities" curve exceeds the safety goal at any point, the repository design would be rejected as not sufficiently safe (see Fig. 2).

FIG. 1. Comparative risks and a probabilistic safety goal.⁽²⁾

FIG. 2. Example of a cumulative probability distribution. The safety goal is chosen by social forces. The predicted performance is unacceptable.

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The abscissa of such a curve can be individual or population dose, for example. The ordinate can be frequency as shown in Fig. 1, or it can be accumulated probability as discussed in Chapter 5 and shown in Fig. 2. There is a transformation, based on the duration of repository performance and frequency of disruptive events, that allows us to go from frequency to accumulated probability.

This paper was written to provide a methodology for calculating a predicted dose curve for a nuclear waste repository like the one in Fig. 2, using a complete set of principal technical uncertainties. The flatness of the central portion of the predicted dose curve, in essence, becomes a measure of how well today's technology can make long-term predictions. If it is too flat, then the technical conclusion should be that the technology must improve before a repository's performance can be ensured. Note that a flat curve does not imply that the system is unsafe, only that the data base is not sufficiently understood to say that it is safe enough.

1.2 CONCEPTUAL ERROR ANALYSIS

Any methodology to predict nuclear waste repository performance is subject to scientific uncertainties in site descriptors, predictive model, future disruptive events, and extrapolation uncertainties.

Scientific calculations consist of both a scientific estimate and a range that indicates the precision of the estimate. The accuracy of the estimate can be measured by how close it comes to its "real" value.

The uncertainty of repository performance predictions can result from problems such as imprecise data, inaccurate data, and invalid modeling. Imprecise data cause prediction uncertainties because the range in values of site descriptor leads to a corresponding range in site performance predictions. The uncertainty in a prediction is dependent on the precision of the prediction. The precision is obtained by propagating uncertainties through the predictive model to the predictions via a Monte Carlo technique (See Fig. 3).

If inaccurate data are used in a valid predictive model, they can result in inaccurate predictions. The inaccuracies in the prediction can be hidden by imprecision in the data.

FIG. 3. Descriptor-induced uncertainty analysis.

Invalid modeling is probably the most insidious of the three problems. It can take the form of incomplete, insufficiently detailed, or erroneous numerical modeling. Incomplete modeling occurs when all the important processes have not been included in a predictive model. Because of the synergistic effects that often occur with various physical processes, extreme caution must be used in dropping off a particular physical process by too simplistic an analysis. Insufficient detail refers to the scientific necessity of choosing a physical size scale of interest, then lumping smaller size-scale phenomena into larger size-scale parameters. In some cases, the effects of smaller size-scale phenomena on larger size scales can be considerable. When this occurs, the choice of size scale can produce inaccurate predictions. Erroneous numerical modeling is not as subtle as the previous two concerns, but sufficient care should be taken to ensure that correct numerical results are generated. Careless formulation of analytical expressions has often led to erroneous and misleading results.

Low-confidence predictive models are easy to generate. High-confidence models require the technical expertise to avoid such dangers as a forgotten process, insufficient detail, or numerical blunders. Invalid predictive models can result in supposedly well-engineered bridges being blown down and buildings collapsing in earthquakes. Obviously, important physical processes were not considered in designing such facilities. To develop high-confidence predictions, careful consideration must be given to both implicit and explicit predictive model assumptions.

1.3 ANALOG ERROR ANALYSIS

Scientific error analysis can give us scientific confidence in our predictions by determining their accuracy and precision. A careful analysis shows whether the accuracy and precision can be improved and where the greatest improvements can be made.

For a good perspective on scientific error analysis, it is instructive to look at a symbolic analog error analysis. By perceiving all of its facets, one can obtain a set of uncertainty concepts applicable to a numerical modeling program.

To this end, we define $H(X)$ as the prediction probability distribution function (PDF) obtained for the set of site descriptors $(X) = (X_1, X_2, \dots, X_n)$. Each subscripted term represents a preferred value and a distribution about the preferred value for one of the site descriptors. H is the symbolic predictor model. The prediction for a baseline case is one-to-one mapping of X_0 to $H(X_0) \equiv H(X_{1,0}, X_{2,0}, \dots, X_{n,0})$. For the sake of this analog discussion, we assume that there is a set of mean descriptors $(\bar{X})$ such that $H(\bar{X}) \equiv \bar{H}$, the mean of the prediction PDF.

The precision of $H(X)$ is found by considering the spread of values from the individual j mappings,

$$H_j = H(X_j) = H(X_{1,j}, X_{2,j}, \dots, X_{n,j}). \quad (2)$$

In the limit of an infinite number of measurements, $N \rightarrow \infty$, the variance of H , which is the square of the standard deviation, σ_H , is

$$\sigma_H^2 = \frac{1}{N} \sum_{j=1}^N (\Delta H_j)^2, \quad (3)$$

where $\Delta H_j = H_j - \bar{H}$ is the predicted deviation of H_j from the mean prediction $\bar{H}$.

The predicted deviations can be expressed in terms of the descriptor deviations by use of a generalized n-dimensional Taylor's expansion about $\bar{X}$,

$$\begin{aligned} \Delta H_k = & \sum_{i=1}^n \frac{\partial H(\bar{X})}{\partial X_i} \Delta X_{i,k} + \frac{1}{2!} \sum_{i=1}^n \frac{\partial^2 H(\bar{X})}{\partial X_i^2} \Delta X_{i,k}^2 \\ & + \sum_{\substack{i,j=1 \\ i \neq j}}^n \frac{\partial^2 H(\bar{X})}{\partial X_i \partial X_j} \Delta X_{i,k} \Delta X_{j,k} + \text{higher order terms}, \end{aligned} \quad (4)$$

where

$$\Delta X_{i,k} = X_{i,k} - \bar{X}_i, \text{ and}$$

$\frac{\partial H(\bar{X})}{\partial X_i}$ means that this partial derivative is evaluated at $\bar{X}$.

If the deviations, $\Delta X_{i,k}$, are small enough, the higher order terms can be neglected; also, to good approximation, the first-order Taylor's expansion, which is linear in the deviations, would be adequate to describe our prediction space. Under these conditions, a sensitivity study would require only $n+1$ computations by H to map the space. This is not the case for repository sites. Thus, if one does not wish to be surprised, the total space must be mapped out, case by case, until one has enough experience to gain a heuristic understanding of the site performance in every portion of the n-dimensional space. As the X_i become large, higher-order terms become important, and correlations between the parameters must be considered. Because many of the parameters such as porosity and permeability are known to be correlated, a simplistic analytical description is likely to result in

misleading predictions. Our only way to determine the precision of the predictions is a Monte Carlo-type investigation on a full-blown numerical model.

If we use the expression for the covariance of X_1 and X_2

$$\sigma_{X_1 X_2} = \frac{1}{N} \sum_{j=1}^N \left[(X_{1,j} - \bar{X})(X_{2,j} - \bar{X}) \right], \quad (5)$$

we get the familiar statistical form of the standard deviation of H in terms of the standard deviations and covariances of the site descriptors,

$$\sigma_H = \sqrt{\sum_{i=1}^n \sigma_{X_i}^2 \left(\frac{\partial H(\bar{X})}{\partial X_i} \right)^2 + 2 \sum_{i=j=1}^n \sigma_{X_i X_j} \frac{\partial H(\bar{X})}{\partial X_i} \frac{\partial H(\bar{X})}{\partial X_j} + \text{higher order terms.}} \quad (6)$$

σ_H and the partial derivatives in this expression are the analogs of the unknowns in numerical sensitivity and Monte Carlo studies. Obviously, two other concerns must be the understanding of the σ_X 's and the validity of H . Assuming that H is valid, one gains greater scientific knowledge when σ_H is reduced. Knowing the partial derivatives and the σ_X 's, one can determine the dominant terms in σ_H . The procedure allows formulation of a strategy that maximizes the rate of reduction in σ_H .

We have assumed that our descriptor space is adequate, but this need not be the case. The descriptor space may not be expansive, realistic, or detailed enough. In particular, the set of n descriptors may need to be expanded to m descriptors, where $m > n$. Three reasons might be, for example, that (1) the salinity of the water must be included in the model; (2) the permeability may have to be made nonisotropic to be realistic, and (3) the microstructure of the sedimentary rock may need to be described in more detail. Such model changes might become necessary as a modeling program progresses. A change in site description would require a reactionary change in the predictive model H or vice-versa. A model change, in turn, could alter the sensitivities of the descriptors and lead to a change in the direction of a technical data base development program.

In summary, improvements in the accuracy of H and the precision, σ_H , in our analog error analysis will occur when: (1) $H(X)$, the prediction space, is mapped out; (2) research is done to reduce or better understand the σ_X 's; (3) research is done to establish more realistic site descriptors; and (4) validations are made of H , the predictive model.

This list of four projects is exhaustive in the sense that complete, high-confidence technical information from our simulation will follow from these efforts. The list implies three closely coupled development efforts for the actual data bases:

1. Development of physically realistic descriptors and their uncertainties. Initially the descriptors are usually generic idealizations.
2. Development of a predictor model that is valid in the descriptor space. Initially only physical processes considered most important are usually included.
3. Mapping of the prediction space to get information of the descriptor sensitivity, the precision of the predictions, and the magnitude of the predictions. This effort enables one to optimally appropriate resources and to improve the data base as quickly as possible.

2.0 DESCRIPTIVE UNCERTAINTIES

2.1 INTRODUCTION

A typical repository description is a complex set of measurable parameters and their uncertainties. Early in a program, assumptions need to be made about the geometry of a repository to provide prediction data. For input data, for example, one might assume that the repository is similar to the conceptual design by Parson et al. (1976).⁽³⁾ Changes in the basic geologic and hydrologic model and/or changes in the assumed conceptual repository design could alter many parameter uncertainties.

Descriptors

In developing the data base for the physical model, uncertainty ranges must be provided for the descriptors. Depending on the results of the initial uncertainty analysis, some of the more sensitive descriptors may be subjected to extensive evaluation and analysis.

For a specific site and assumed level of exploration and instrumentation, uncertainty at a given level would be associated with each parameter. Uncertainty arises from geologic variations, errors in and limitations of testing techniques, and limitations in the evaluations of the tests or explorations. Different levels of exploration lead to different levels of uncertainty. In past studies,⁽⁴⁾ we have considered for the preconstruction phase, for example, the following general exploration levels as appropriate:

- Minimal: No boreholes but research of available regional information and surface mapping
- Moderate: Approximately 40 shallow holes to the level of the repository and 10 deep holes through to underlying aquifers.
- Maximum: Extensive explorations with hydrologic testing.

Uncertainty values are expressed in terms of confidence limits on the median value. For example, if the 90 percent confidence limits for a parameter are A and B, it means that if the parameter were repeatedly sampled,

then 90 percent of the time the value obtained would lie between A and B. The geotechnical parameters were initially assumed to fit a modified lognormal distribution. The standard unit for defining the uncertainty, U, of a parameter would correspond to one standard deviation in the logarithm of the parameter. For the lognormal distribution, if the value of the parameter is V, the definition of its uncertainty, U, is that approximately two-thirds of the sample population of the parameter lies between V/U and VU, or alternatively, 95 percent of the sample population lies between V/U² and VU². All our uncertainty values are then given in terms of the value U and the maximum and minimum values of the parameter. Our "best estimate" is V, the median of the lognormal distribution.

2.2 HANDLING DESCRIPTIVE DATA

Distribution of Parameter Values

The statistical distribution shown in Fig. 4 seems appropriate as a starting point to describe the uncertainties in most descriptive parameters. This description (derived from a lognormal distribution) is defined by

$$P(V, V_{\min}, V_{\max}, U) = \frac{N(V_{\min}, V_{\max})}{V \sqrt{2\pi} \ln U} \exp \left\{ -1/2 \left[\frac{\ln(V/V_{1/2})}{\ln U} \right]^2 \right\} \quad (7)$$

where:

- U = geometric standard deviation of parent lognormal distribution
- V = value of descriptive parameter
- V_{min} = minimum plausible value of V
- V_{max} = maximum plausible value of V
- V_{1/2} = median value of parent lognormal distribution
- N(V_{min}, V_{max}) = normalization factor.

The distribution is normalized so that

$$\int_{V_{\min}}^{V_{\max}} P dV = 1. \quad (8)$$

FIG. 4. Distribution used to describe the range of values for descriptive parameters.

This distribution is especially convenient when uncertainties range over several orders of magnitude, and when it can be justified physically. The physical justification assumes that, unless descriptive parameters are very accurately specified ($U \ll V_{\max}/V_{\min}$), one well-behaved distribution is as good as another, as long as it spans an adequately large range of parameter values (see Fig. 5a). When the descriptive data are very precise, we can either continue to use the skewed distribution described in Fig. 4, and assume that other uncertainties will overwhelm any errors introduced by its skewedness, or if necessary we can substitute a more symmetrical distribution (see Fig. 5b). The relative values of the variables that describe the distribution determine its general shape and can be used to arbitrarily define three increasingly sophisticated levels of analysis. Figure 6 illustrates typical shapes and lists the characteristics of each of these levels.

The first level depends only on expert opinion (based on available data) for the median parameter value ($V_{1/2}$), the credible range of parameter

FIG. 5. Effect of data base size on the statistical distribution. In (a), where few measurements have been made and the data are scattered, either of the distributions shown will suffice, provided that it adequately covers the entire range of plausible parameter values. In (b) the data are precise enough to distinguish between alternative distributions.

FIG. 6. Three levels of analytical effort. Each can be described by the relative values of the variables used to define the probability distribution and by several general characteristics. The uncertainty in the hazard prediction decreases as the descriptive information improves.

values (bounded by $V_{\min}$ and $V_{\max}$), and the value of the parameter (U) that specifies the breadth of the parent distribution. At this stage of analysis, the range must encompass all plausible values for a generic site, and the value of U chosen is very large. The result is a flat, featureless distribution function covering the range of possible parameter values.

The second level of analysis corresponds to a phase of exploration and data gathering. It depends on better data for each generic site and is characterized by a more confident estimate of $V_{1/2}$, a smaller value for U , and a smaller range of plausible parameter values. At this level, the distribution function for a given parameter still cannot be regarded as rigorously quantitative, because the analysis depends not only on an incomplete data base but also on expert judgment.

The third stage culminates the evolution from informal analytic methods to a formal, inductive technique. It requires a substantial body of carefully analyzed data, that can be put in an appropriate mathematical form. A physical model for the parameter must then be developed using regression analysis. This level of analysis demands a thorough understanding of exploratory techniques and uncertainties, of relevant physical processes, and of laboratory analytical methods. The result is a still more confident estimate of the descriptive parameter. Because this final stage demands considerable resources, it is practical only for some descriptive parameters where more accurate analysis is likely to improve substantially the confidence of hazard forecasts.

Parameter Correlations

When establishing the uncertainties of descriptive parameters, it is important to recognize that some parameters may be closely correlated. An example is the permeability and porosity of rock. If this correlation is ignored when making forecasts for generic sites (where parameter uncertainties are considerable), we would unduly emphasize the unrealistic situations where permeability is high and effective porosity low. The high permeability would lead to the calculation of a relatively high radionuclide flux, and the low porosity would demand that this flux be translated into a very high radionuclide velocity. The result would be an unrealistically high estimate of the potential hazard.

It can be illustrated schematically how pairs of parameters might be correlated. Where sufficient data are available, quantitative distributions are useful for quantifying such correlations. At the left of Fig. 7, descriptive parameters V_1 and V_2 are uncorrelated; the illustrations to the right show an increasingly stronger relationship between the two parameters.

FIG. 7. Range of correlations between descriptive parameters.

Interpolation as a Source of Data

In some cases, data may not be available for a descriptive parameter for a site being analyzed. However, if a tested physical model exists that relates the needed parameter to known parameters, the data can be inferred rather than directly measured. In many cases, this amounts to interpolating between experimental results relating parameters using a numerical formulation like that shown in Fig. 8. Such interpolations carry with them rigorous statistical distributions. In this example, the data fit a curve described by

$$V(W) = \frac{a}{W^b} \quad (9)$$

The uncertainties in the constants a and b can be calculated by regression analysis, and a new parameter value shown in Fig. 8, $V(\tilde{W})$, evaluated as

$$V(\tilde{W}) = \frac{a \pm \Delta a}{\tilde{W}^{b \pm \Delta b}} \quad (10)$$

Once models like the one in Fig. 8 have been developed and inferences made, we can accurately judge whether additional measurements should be made to ensure greater confidence in inferred values. For example, in Fig. 8, an experimental measurement of V at W' would greatly decrease the uncertainty of inferences in the vicinity of $\tilde{W}$.

FIG. 8. Derivation of descriptive parameters by inference. If a physical model can be reduced to a numerical formulation on the basis of known data, further parameter values can be inferred by interpolation. This curve also suggests that a measurement of V at W' would significantly improve our confidence in inferences of $V(\tilde{W})$.

3.0 DYNAMICAL UNCERTAINTIES

3.1 INTRODUCTION

The term predictive model, as used here, refers to the governing physical laws that dictate the time evolution of the hazardous radionuclides in the repository, their analytical and numerical form, and the simplifying assumptions needed to put them into usable form. It also refers to the physical size scale used to model the repository. The computational form of the predictive model for the repository must be numerical, as the time evolution of the system is too complex to solve in closed analytical form.

An ongoing program must be part of any modeling effort that ensures that the model will be realistic enough to make credible predictions. Simplifying and expediting assumptions that are necessary to generate timely predictions must be evaluated to develop model credibility.

The final believability of a model is determined by its ability to predict actual doses. Clearly, for a repository that must function far into the future it is impossible to provide timely predictions from a validated model if comparison with actual doses is the only acceptable validation procedure. However, there are other ways to gain confidence in a predictive model. For example, one can verify subsystems of the model and test some of the physical and numerical assumptions and processes. This process will lead to a model with an increased confidence level.

Lack of confidence in a predictive model comes usually from uncertainty in the model structure; a secondary source of uncertainty is numerical. Unless one carefully considers such things as numerical roundoff error, truncation error, and formulation of analytical expressions, the transformation of an analytical model into a numerical model can lead to disastrous errors. Moderate caution, however, can usually minimize computational problems.

The predicted dose to humans from a typical waste repository is based on parametric simulation models for radionuclide inventory, groundwater waste migration, and dose intake. Migration models have been used to predict repository performance for relatively simple geological and hydrological scenarios, and a substantial effort is being made to expand their capabilities

and improve their acceptability. Models with insufficient complexity are known to produce inaccurate predictions, and yet a too-detailed model may be too specific for one's purposes. The modeler must ensure that a balance between too little and too much detail is met.

Factors such as thermal gradients, variable fluid densities, and long-range climatic changes, which have been neglected in many of the models, may radically affect groundwater flow regimes. The importance of these effects should be evaluated, along with the technological limitations on their treatment. Under some conditions, the steady-state hydrology model may not be appropriate, and transient hydrological modeling may be necessary. If so, the modeling capabilities should also include a time-dependent hydrological model.

3.2 MONTE CARLO PREDICTION UNCERTAINTIES

A subsurface waste migration model is characterized by such geological and geochemical parameters as permeability and porosity of the geological components and retardation factors for the various nuclides. The assumed parameter values used in risk calculations are uncertain for a number of reasons, including measurement uncertainty, which is a function of level of exploration. Uncertainty in the data parameters should give rise to uncertainty in the site performance predictions. The approach taken here is to specify the underlying model values and their ranges in terms of probability distribution functions, as discussed in Chapter 2. A Monte Carlo computer program can be developed to generate a set of random parameter values using specified probability distributions. These parameters are used as input to the program which simulates the flow of waste out of a repository. Each set of parameters represents a possible configuration of geological and geochemical characteristics for the repository. This process is repeated for a number of parameter sets (say 50); statistical analysis may then be performed on the ensemble of outputs.

The Monte Carlo approach to the uncertainty analysis facilitates a statistical characterization of the prediction uncertainty. The technique, which is simple to implement, is flexible in that it can be modified to accommodate a wide variety of descriptor distributions and constraints. A drawback is the possibly large amount of computer time needed to perform.

enough Monte Carlo trials to represent the tails of the parameter distributions adequately. Where the budget does not permit a large number of trials, an alternative method of extrapolation to low-probability events can be implemented. We describe such a method in Chapter 5.

3.3 MODEL DESIGN

The probabilistic model that predicts the future behavior of buried waste must yield accurate and technically defensible results, quantify the uncertainties, and yet be simple enough to be computationally tractable. We have sought in the past to achieve these goals by using a three-tier approach illustrated schematically in Fig. 9. The central feature of the scheme is the predictive model itself (tier 2), which is based initially on the approximations and insights afforded by the rough models of tier 1. At first, the predictive model can be thought of as being well to the left in Fig. 9, where its defensibility is low. As the program progresses, tier 3 provides state-of-the-art models to test the assumptions in the predictive model and to supply rigorous numerical inputs. Using feedback from both tiers 1 and 3, the model migrates to the right, toward greater scientific defensibility.

In addition to the general design of the computational scheme in Fig. 9, a second means of improving model efficiency is to provide, whenever possible, input data in the form of scaling sets. For example, where a single flow path is the dominant barrier to the biosphere, the travel time across the flow path for the center of the radioactive pulse is given by

$$t_e = \frac{z^2 \phi K_f}{kp} \quad (11)$$

where

- z = length of flow path
- ϕ = effective porosity
- K_f = retardation factor
- k = hydraulic conductivity
- p = driving pressure.

FIG. 9. Schematic illustration of the probabilistic model used to predict the future behavior of buried waste. The process starts with approximate models, which provide initial insights and increase its defensibility by the use of state-of-the-art models, which provide tests of assumptions and approximations. This three-tier approach ensures that the model is both accurate and computationally efficient.

Assuming that longitudinal dispersion can be accounted for separately, an analysis need consider only a range of values for t_e (rather than z , ϕ , K_f , k , and p separately). These five descriptive parameters, interrelated as shown, constitute a scaling set. These scaling sets not only reduce the amount of computer time required for an analysis (by simplifying the input), but also provide insight into the tradeoffs among descriptive parameters.

4.0 DISRUPTIVE EVENT UNCERTAINTIES

4.1 INTRODUCTION

Prediction of radiation doses resulting from a waste management system involves consideration of a sequence of probabilistic events. In addition to uncertainties in the dynamic models and in the descriptive parameters, we must account for uncertainties caused by events we cannot model deterministically. Among stochastic events that should be considered in any long-term risk analysis are breccia pipe formation, backfill failure, climatic changes, meteor strikes, earthquakes, and social changes.

Some catastrophes, such as meteor strikes, occur unpredictably with a constant frequency; however, the frequency of other nondeterministic events, especially those associated with social and political activity, varies with time. Figure 10 illustrates several examples, based on the following three assumptions:

- The frequency of canister failure is initially zero, but increases to a large value over a period of many thousands of years.
- The political climate improves so that the prospect of a nuclear bomb strike and prospect of terrorist intrusion decrease to near zero in about 100 years (a very optimistic assumption).
- Administrative policing of the site initially ensures against accidental human intrusion, but the risk of intrusion increases with time. The time at which risk becomes appreciable depends largely on the public perception of the need to continue policing the site and on government stability. (This variability is illustrated by the display of two curves for accidental human intrusion in Fig. 10.)

We can gain further insight into the consequences of these time-dependent events by evaluating the hazard in several specific scenarios. In Fig. 11 the five curves hypothetically represent the hazards that would result from accidental human intrusion at the five times indicated on the abscissa. Plots such as these indicate the time during which the integrity of the site should be maintained.

FIG. 10. Frequencies of several time-dependent catastrophic events. These are compared with constant frequencies of meteor strikes and earthquakes. The assumptions that underlie the time-dependent curves are discussed in the text, as are the factors that influence the curves for accidental human intrusion.

FIG. 11. Consequences of human intrusion for five different scenarios. The five curves illustrate the hazard that would result from accidental human intrusion at five times indicated on the time axis. The error bars represent the uncertainties in each hazard estimate. To avoid risk of a hazard that exceeds the established safety standard, integrity of the site should be ensured during the time indicated by the crosshatched area.

4.2 SINGLE DISRUPTIVE-EVENT CURVES

In addition to considering the probability of disruptive events, one must evaluate the probability of resulting dose levels, given that a disruptive event has occurred.⁽⁵⁾

For a single disruptive event E_i assumed independent of other disruptive events, let

$P(D', t | E_i, t')$ = Conditional probability distribution function (12)
of dose greater than D' at time t given the
occurrence of event E_i at time t' .

When $P(D', t | E_i, t')$ is determined over a suitable range of doses and times, it is possible to plot maximum individual doses as a function of time and probability. Systematic analysis of the consequences of a given disruptive event on a geologic repository, for example, might result in a family of curves as illustrated in Fig. 12.

FIG. 12. Sample dose-time-probability relationship.

To illustrate the method, let us assume that the post-emplacment analysis of a given repository yields the results of Table 1. From such data, it is possible to plot the probability versus dose relationship shown in Fig. 13. It should be noted that the time at which a given maximum dose level is reached is not considered. This specifies that dose level importance is independent of time of occurrence of the dose level, i.e., zero time discounting is used.

TABLE 1. Post-emplacment dose example for E_1 occurring at t' .

Probability $P(D')$	Maximum lifetime dose D' (rem)
9×10^{-2}	10^{-2}
3×10^{-3}	10^{-1}
2×10^{-4}	1.0
2×10^{-6}	10
2×10^{-8}	100
2×10^{-12}	1000

Having plotted the predicted probability-dose relationship, a safety goal can be displayed in Fig. 13. Because all predicted values in this example fall below the safety goal, the system would be judged acceptable.

Another example to illustrate pre-emplacment operation is indicated in Table 2. We assume that a probabilistic model predicts these results. The dose-probability curve can be plotted as shown in Fig. 14. By superimposing the safety curve for maximum annual dose, it can be seen that the probabilistic safety goal is exceeded at low probability levels. This waste management system would be rejected.

TABLE 2. Pre-emplacment dose example.

Probability P(D)	Maximum annual dose D' (rem)
3×10^{-2}	10^{-2}
5×10^{-3}	10^{-1}
5×10^{-4}	1
6×10^{-5}	10
4×10^{-6}	100
8×10^{-8}	1000

4.3 MULTIPLE DISRUPTIVE EVENTS AND OTHER UNCERTAINTIES

Traditional assessments have mostly dealt with only disruptive-event uncertainties and probabilities. Constraining ourselves to assessments with only disruptive-event uncertainties provides a focus that is too narrow for dealing with repository predictions. For a deep geological repository, the dominant uncertainties are most likely descriptor uncertainties (see Eq. 1). If this is borne out by analysis, these uncertainties will determine to good approximation the risk curve shown in Fig. 2. The other uncertainties will modify this curve only slightly. Descriptor uncertainties are mainly caused by the difficulty of describing the detailed transport features of a deep geological formation.

In the previous section we considered the probability that the dose D' to an individual is exceeded when the site undergoes a single disruptive event. No descriptive or predictive uncertainties were considered. This section deals with sequences of disruptive events as well as descriptive and predictive model uncertainties. The parameters in this section are mathematically represented by:

- $K_D(t)$ = Time-dependent site description parameter sets (spans descriptor uncertainties)
- K_P = Prediction model parameter sets (spans predictor uncertainties)
- K_E = Disruptive event parameter sets (spans event uncertainties).

FIG. 13. Post-sealing dose versus accumulated probability.

FIG. 14. Sample dose-probability relationship for pre-emplacment operations.

The only principal uncertainty not included in this chapter's discussion is tail-extrapolation uncertainty. A method for handling this uncertainty is discussed in Chapter 5.

4.4 FORMALISM INCORPORATING THREE UNCERTAINTIES

For the sake of this discussion, a discrete-variable probability format will be used. It is a trivial matter to incorporate a continuous variable description. However, even if a continuous description were used, a discrete description would be necessary for the numerical simulation.

Let K be the set of all possible parameter realizations for a specific repository. In terms of the parameters described above, $K = \{K_D, K_P, K_E\}$, a triad of groups of parameters describing the site features, the dynamical model, and the disruptive events, respectively. To obtain a numerically tractable problem, the set of possible parameters must be segmented into subsets. Each subset, K_i , is represented by a typical value of the parameters, K_i^x , and a probability that subset K_i will be realized, $P(K_i)$ (see Fig. 15). To determine $P(K_i)$ it is necessary to do analyses, including Monte Carlo calculations, to determine how often the parameters in each domain occur.

FIG. 15. Schematic of the subsets of parameters. Selection of the parameters at point x of each subset will lead to a forecast not significantly different from any other selection in the subset.

For each K_i^x there is a deterministic individual dose as a function of time shown in Fig. 16 that is realized, $d_{K_i}^x(t)$. The domains for K_i are chosen so that any choice from within K_i will not significantly alter $d_{K_i}(t)$, i.e., $d_{K_i}(t) \approx d_{K_i}^x(t)$.

We now want to formulate the program for determining the probability so that no individual will receive greater than a specified dose D' . In this regard, if only one future individual receives greater than dose D' from parameter set K_i , the probability that K_i is realized, $P(K_i)$, is added to the probability that D' is exceeded. Formally, the probability that D' will be exceeded, is

$$P(D') = \sum_i P(K_i) \eta(\hat{d}(K_i); D'), \quad (13)$$

where the "tally operator" is defined as

$$\eta(\hat{d}(K_i); D') = 1, \text{ if } \hat{d}(K_i) > D' \quad (14)$$

= 0, otherwise; and,

$\hat{d}(K_i)$ is the peak dose that occurs for the parameter subset K_i . The summation is over all K_i ; that is, the index i runs over all possible subsets (see Fig. 15).

4.5 DISRUPTIVE EVENT PERTURBATION APPROACH

Disruptive events are defined here as significant physical processes which lead to a different geological state of the site. They are not predictable, and are assumed independent of other disruptive events. If a disruptive event occurs, its impact on the geological/hydrological state of the site is assumed known. The frequency of the event is also assumed known to good approximation.

FIG. 16. Individual dose versus time for a scenario represented by parameters K_i .

In a well-sited repository, it is expected that disruptive events will have a low probability of occurrence during the time that the waste requires containment. This low probability of occurrence, coupled with the concept of sequences of disruptive events, suggests a perturbation approach to the prediction problem. A summation of probability terms, with each addend representing one more disruptive event occurring during the containment period than its predecessor, would have decreasing probabilities for each successive addend. This lends itself to a perturbation approach to risk analysis. Let us define the i^{th} time-ordered sequence of N disruptive events during the time span τ by the set of parameters

$$\{K_E^{(N)}\}_i = \{(t_1, E_1), (t_2, E_2), \dots, (t_j, E_j), \dots, (t_N, E_N)\}_{j_i}, \text{ and} \quad (15)$$

$$t_1 \leq t_2 \leq \dots \leq t_j \dots \leq t_N < \tau$$

where t_j represents the time at which the j^{th} disruptive event occurs, E_j is the j^{th} disruptive event, and the i index represents one of the many sequences possible with N events. The time period during which the repository must operate safely is τ .

Let $P^{(N)}(D')$ be the probability that N disruptive events occur and the outcome is a maximum dose greater than D' . Then, ignoring the descriptive and predictive model uncertainties, we can write

$$P^{(N)}(D') = \sum_i P\{K_E^{(N)}\}_i \eta(\hat{d}\{K_E^{(N)}\}_i; D') \quad (16)$$

where $P\{K_E^{(N)}\}_i$ = probability that the sequence of events $\{K_E^{(N)}\}_i$ is realized, and η is the tally operator defined in Eq. 14.

Because we know that some number of disruptive events will occur, including the possibility of no events, we have completeness

$$1 = \sum_{N=0}^{\infty} P^{(N)}(n'=0) \quad (17)$$

For $D' > 0$, the summation is less than 1.

If we only want to consider sequences or events with less than or equal to L events, we can write

$$P_L(D') = \sum_{N=0}^L P^{(N)}(D') \leq 1 \quad (18)$$

where

$$P^{(N)}(D') = \sum_i P\{K_E^{(N)}\}_i \sum_D P(K_D | \{K_E^{(N)}\}_i) \sum_P P(K_P) \eta(\hat{d}(i, N, D, P); D'); \text{ and} \quad (19)$$

$\hat{d}(i, N, D, P)$ is the peak dose for the sequence of N events specified by i , descriptive parameters K_D , predictive parameters K_P , and L is the order of the perturbation calculation. Also, Eq. (19) includes the terms for the predictive model and descriptive uncertainties not included in Eq. (16).

Notice that the site description is assumed dependent on the sequence of disruptive events. However, the model of how the various components interact, i.e., the physical laws governing the interaction of the parts, is assumed not to depend on the sequence of disruptive events.

The perturbation approach for truncating the analysis will be useful if both

$$(1) \quad p^{(N+1)}(D) \ll p^{(N)}(D'), \text{ and} \quad (20)$$

(2) social values are such that events with a sufficiently low probability of occurrence can be ignored in the risk assessment.

If these conditions are met for $p^{(N)}(D')$ sufficiently small, no analysis is required for greater than or equal to N sequential disruptive events. The plot of the results of such an analysis would look something like Fig. 17. If the curve $p^{(N+1)}(D')$ crossed $p^{(N)}(D')$ below a probability of, say, 10^{-8} , then there could be a rule to discontinue any higher order calculations. This would provide a well-defined technical scheme to truncate resources spent on numerical analyses.

If the effect of disruptive events is small compared to the effect of descriptors, then there is probably no point in doing many calculations using different disruptive events at different times. Mathematically, the case where the uncertainties in the descriptors are overwhelming can be written

$$P(D') \approx p^{(0)}(D') \text{ to sufficiently low probabilities.} \quad (21)$$

Thus, we have two methods to truncate the disruptive-event calculation:

- (1) if probability is less than some sufficiently small number, or
- (2) if the dose is insensitive to a particular disruptive event.

For case (1), there might be a high consequence, but it is considered too improbable to worry about. For case (2), the probability might be very high for disruptive-event occurrence, but the results will not be significantly different than if the event did not occur. In the second case the subset of the total parameter space containing this event would be reduced by elimination of this event from consideration, thus slightly decreasing $p^{(N)}(D')$ where $N \geq 1$, but increasing $p^{(0)}(D')$.

FIG. 17 Dose accumulative distributions with 0, 1, 2, and 3 disruptive events. Also shown is the total dose accumulative distribution function obtained from an L^{th} order perturbation calculation.

An Example

Let us pursue the notation and ideas in this chapter a bit further with an example. From Eq. 19, for a single event scenario, we can write

$$p^{(1)}(D') = \sum_i P\{K_E^{(1)}\}_i \sum_D P(K_D | \{K_E^{(1)}\}_i) \sum_P P(K_P) n(\hat{d}(i, 1, D, P); D') \quad (22)$$

If the physical laws are given uniquely (no uncertainty range in predictive model parameters), or if $\hat{d}$ is insensitive to the choice of K_P 's, then

$$p^{(1)}(D') = \sum_i P\{K_E^{(1)}\}_i \sum_D P(K_D | \{K_E^{(1)}\}_i) n(\hat{d}(i, 1, D); D') \quad (23)$$

If there is only one type of disruptive event that is significant in its effect, then the label i refers to its time of occurrence only.

$$p^{(1)}(D') = \sum_i P(t_i^{(1)}) \sum_D P(K_D | t_i^{(1)}) \eta(\hat{d}(t_i^{(1)}, 1, D): D') \quad (24)$$

where $P(t_i^{(1)})$ is the probability that the event occurs only once during τ and at time t_i .

If no matter when the event occurs, the set K_D remains essentially unchanged, then remembering that D refers to the set of descriptive parameters and D' refers to the dose, we can write

$$P(K_D | t_i^{(1)}) \equiv P(K_D) \quad (25)$$

and

$$\eta(\hat{d}(t_i^{(1)}, 1, D): D') \equiv \eta(\hat{d}(1, D): D') \equiv \eta(\hat{d}(D): D') . \quad (26)$$

If the rate of occurrence for the disruptive event is Λ , and the time interval for containment is τ , then the probability of occurrence during τ for $\tau\Lambda \ll 1$, is

$$1 - (1-\Lambda)^\tau \approx \tau\Lambda . \quad (27)$$

Thus, rewriting Eq. 19 for this limited case, we get

$$p^{(1)}(D') = \sum_i P(t_i^{(1)}) \sum_D P(K_D) \eta(\hat{d}(D): D') . \quad (28)$$

Then

$$p^{(1)}(D') \approx \tau\Lambda \sum_D P(K_D) \eta(\hat{d}(D): D') . \quad (29)$$

A similar analysis would show

$$P^{(2)}(D') \approx (\tau\Lambda)^2 \sum_D P(K_D) \eta(\hat{d}(D):D') \quad . \quad (30)$$

If D' is sufficiently small that

$$\sum_D P(K_D) \eta(\hat{d}(D):D') \approx 1 \quad , \quad (31)$$

then using induction we can write

$$P^{(N)}(D') \approx (\tau\Lambda)^N \quad . \quad (32)$$

Thus, for the assumptions we have made for this case and times of interest τ and rates of occurrence Λ such that $\tau\Lambda \ll 1$,

$$\frac{P^{(N+1)}(D')}{P^{(N)}(D')} \approx \tau\Lambda \ll 1 \quad . \quad (33)$$

This example implies that some simple probability analysis of the disruptive events might exclude many multiple disruptive events from the analysis. Using the fact that

$$P^{(N)}(D') < (\tau\Lambda)^N \text{ since } P^{(N)}(D') < P^{(N)}(0) \quad , \quad (34)$$

and assuming, for example, that

$$\tau = 10^6 \text{ years and } \Lambda = 10^{-9} \text{ yr}^{-1}, \text{ and} \quad (35)$$

10^{-8} probability is considered an "improbable event," i.e., so rare as to not be of concern, then

$$P^{(N)}(D') < 10^{-9}, \text{ if } N \geq 3 \quad . \quad (36)$$

Therefore, at most, a third-order perturbation study would be in order for this case. We would only need to calculate the summation

$$P_3(D') = \sum_{N=0}^3 P^{(N)}(D') . \quad (37)$$

This knowledge would be useful in planning and carrying out a program to predict the long-term safety of a repository.

5.0 TAIL-EXTRAPOLATION UNCERTAINTIES

The first three uncertainties we discussed in Chapters 2, 3, and 4 are caused essentially by limitations on data gathering and analysis capabilities. This inherently limits our ability to forecast repository performance. The fourth uncertainty, i.e., the low-probability tail uncertainty, is caused by limitations in computer technology. If we had infinitely fast computers, this tail-extrapolation uncertainty would disappear. Because capabilities of computers are limited, costs for a large number of runs usually become prohibitive; thus, the random sampling of predictive models by Monte Carlo methods will not usually allow description of very low-probability tails.

Figure 18 shows the results of an actual Monte Carlo simulation of 50 trials for a shale repository. The shaded histogram is the probability density function with six bins per decade. The peak individual dose is defined as the maximum dose received by an individual in the future. To generate this curve, a set of parameters is randomly chosen from appropriate distributions representing the data obtained at a generic shale repository. Each choice of a parameter set leads to a result by means of a deterministic numerical model.

When only 50 runs are made, the tail of the distribution is only developed to about a 10^{-2} accuracy. This is shown in Fig. 19 as the hatched histogram. To extend the tail another decade to 10^{-3} accuracy, 500-2000 calculations would be required. Likewise, to obtain a decent representation of the tail by sampling at 10^{-8} accuracy would require $\sim 10^8$ samples. At one second per calculation, this would take about three years to complete, running the computer continuously. Such accuracy, of course, requires great confidence in the model, and might be justified if one had a well-established, fast-running model and a large budget to run the computer.

If decision makers are satisfied with information on events only having one chance in 100 of occurring, then the results in Fig. 18 are probably accurate enough. However, if one wants to know the consequences of scenarios that have $\sim 10^{-8}$ chance of occurrence, then a method must be devised to extrapolate the curve. This can be done by making funding available to run the computer for the number of trials necessary, or by doing curve fitting.

FIG. 18. Shale repository risk curve.⁽⁶⁾ There is 6×10^6 MWe-yr of waste in the repository.

FIG. 19. Probabilistic evaluation of dose from repository.

A traditional approach to curve fitting and extrapolation is to do regression analysis against the data frequency distribution, e.g., the distribution shown as the shaded area in Fig. 18. Care must be made in choosing the regression model. The subjective choice of extrapolation model is extremely important in regression analysis. The extrapolation is sensitive to model choice. Different models can be tried, and the best chosen. If the needed results are robust to different choices, the choice of model is not critical. However, if the decision on the system safety appears marginal with respect to model choices, then more computer runs of the model might be necessary to establish better the distribution and statistically to show that one extrapolation model is preferable.

For example, two good choices to extrapolate the results shown in Fig. 18 are the lognormal distribution and the bimodal lognormal distribution. This is because the uncertainties in the model are so large that the abscissa is, of necessity, a logarithmic scale. Because it is reasonably symmetric about $\sim 5 \times 10^{-6}$ rem, a single-mode lognormal distribution with two parameters might be proposed as the "best" model. Mathematically, it is given as

$$p(D) = \frac{1}{\sqrt{2\pi} D \ln \sigma} e^{-\left(\frac{\ln D - \ln \bar{D}}{\sqrt{2 \ln \sigma}}\right)^2}, \quad (38)$$

where:

- D = the peak individual dose.
- σ = the geometric standard deviation.
- $\bar{D}$ = the geometric mean, and
- $p(D)$ = the peak individual dose probability density function.

Another model suggested by Fig. 18, because it is not completely symmetric, is the bimodal lognormal distribution. This is a five-parameter model. Its form is

$$p(D) = \frac{(1-A)}{\sqrt{2\pi} D \ln \sigma} e^{-\left(\frac{\ln (D/\bar{D}')}{\sqrt{2 \ln \sigma}}\right)^2} \quad (39)$$

$$+ \frac{A}{\sqrt{2\pi} \bar{D} \ln \sigma} e^{-\left(\frac{\ln(D/\bar{D})}{\sqrt{2 \ln \sigma}}\right)^2}.$$

The parameters to be fit are A , $\bar{D}'$, $\bar{D}$, σ , σ' .

The symbol A is a normalization factor so that

$$\int_{-\infty}^{\infty} p(D) dD = 1.$$

Studies using both models will give the decision maker a feeling for how important the choice of regression model is.

We will assume for the sake of this discussion that the two-parameter lognormal distribution is proved the best model. A weighted regression is made, with each bin in Fig. 18, for example, having a variance of n , where n is the number of counts in the bin.

The results of the regression are values and uncertainties for the two parameters in Eq. 37, i.e.,

$$\sigma = \langle \sigma \rangle \pm \Delta \sqrt{V(\sigma)} \text{ and,} \quad (40)$$

$$\bar{D} = \langle \bar{D} \rangle \pm \Delta \sqrt{V(\bar{D})}$$

where $\langle \sigma \rangle$ and $\langle \bar{D} \rangle$ are the best fits and $V(\sigma)$ and $V(\bar{D})$ are the variances of σ and $\bar{D}$, respectively.

The covariance and goodness-of-fit indicators are also available to provide information on how good the regression model choice is. If the fit appears to be a good one, then the extrapolation determines the "best estimate," i.e., the 50th percentile curve, of the low-probability tails. However, if one uses the 90th percentile curve, i.e., the fit for which there is a 90 percent chance that the extrapolation curve is to its right, then the conclusions on dose levels can be quite different from the "best-estimate" curve.

The upper and lower curves shown in Fig. 20 indicate how the predictions can differ.

As one increases the number of trials used to generate Fig. 20, the difference between curves diminishes. For about 100 trials, the relative standard deviations of σ and $\bar{D}$ are about 10 percent.

Because of the steepness of the curve at high consequences, the prediction of the probability of occurrence of a dose can be substantially different, based on the choice of curves in Fig. 20. Table 3, column 4, indicates the interpretation problem which occurs. Depending on how we choose our "best fit," we can interpret the probabilities in different ways. This ambiguity is a result of the tail-extrapolation procedure. The more computer runs that are made, the less ambiguity.

TABLE 3. Comparison of interpretations of curves in Fig. 20.
Note the ambiguity that can result.

Curve confidence level	Probability		
	real curve to the right of plotted curve	What curve indicates about 10^{-4} rem dose	Probability dose 10^{-4} rem exceeded
50%	0.5	Probability that 10^{-4} rem is ex- ceeded is 10^{-4}	0.5×10^{-4} = 0.00005
90%	0.1	Probability that 10^{-4} rem is ex- ceeded is 10^{-2}	0.1×10^{-2} = 0.001

A method for resolving this ambiguity is suggested schematically in Fig. 21. This schematic can be drawn for two parameters. For n parameters, it becomes an n -dimensional problem that can be handled numerically but not depicted graphically.

FIG. 20. Comparison of two tail-extrapolation curves. One is at 50 percent confidence level and the other at 90 percent confidence level.

FIG. 21. Dose probability distribution function, $P_T(D)$, including tail-extrapolation uncertainties.

Figure 21a shows a grid of probability bins associated with realizing $(\bar{D}_i, \sigma_j)$. Discretized values of $\bar{D}$ range from $\bar{D}_0$ to $\bar{D}_m$, and for σ from σ_0 to σ_n . The probability of seeing the combination of $(\bar{D}_i, \sigma_j)$ as the correct values of the geometric mean and standard deviation is P_{ij} .

If the correlation between $\bar{D}$ and σ is zero, P_{ij} is given by

$$P_{ij} = \left[\int_{\bar{D}_{i-1}}^{\bar{D}_i} p(\bar{D}) d\bar{D} \right] \left[\int_{\sigma_{j-1}}^{\sigma_j} p(\sigma) d\sigma \right]. \quad (41)$$

Where the correlations between $\bar{D}$ and σ are sufficiently large, the correlations must be taken into account in establishing the P_{ij} 's.

The choice of grid size and the number of bins (i.e., $m \times n$) are dependent on the accuracy that one needs for the tails. The resulting final curve $P_T(D)$ shown in Figure 21b should not be dependent on the choice of range and mesh size. The range should be made sufficiently large and the mesh size sufficiently small to accommodate tails of $P_T(D)$ to as low a probability as needed.

Once the P_{ij} 's are established, a weighted numerical integration of

$$p_{ij}(D) = \frac{1}{\sqrt{2\pi} \bar{D} \ln \sigma_j} e^{-\left(\frac{\ln D - \ln \bar{D}_i}{\sqrt{2 \ln \sigma_j}} \right)^2} \quad (42)$$

can be made.

The result is shown in Fig. 21b as

$$P_T(D) = \sum_{i,j=1}^{m,n} P_{ij} \cdot p_{ij}(D). \quad (43)$$

This is the dose density function that includes the principal technical uncertainties in the problem, including the tail-extrapolation uncertainty.

If $P_T(D)$ is only a small change from the density function given by the "best-fit" result (see Fig. 22), then one can conclude that the uncertainty introduced by the finite number of computer runs (50 trials, for example) is

small compared with other uncertainties. Under these circumstances, a larger number of computer runs would not improve the uncertainties in the problem in a significant way. In fact, the "best-fit" curve derived from the three uncertainties described in previous chapters should give adequate results.

The utility of incorporating tail-extrapolation uncertainties must be determined for each problem. For problems like the waste repository with inherently large measurement uncertainties, going through the exercise depicted schematically in Fig. 21 will probably show that little can be gained in precision by a large number of computer trials. On the other hand, problems with very little data uncertainty will have results very sensitive to the number of computer trials. In such cases, it would be appropriate to increase the number of trials.

Figure 22 schematically demonstrates the differences between $p(D)$ and $P_T(D)$. If these curves are insufficiently different to impact the decision for which they were derived, then incorporation of the tail-extrapolation uncertainties can be ignored. Conversely, when they are substantially different, the tail-extrapolation recipe prescribed here should be used if a larger number of trials is prohibitively costly. This, however, is not a substitute for the quality of the results obtained by doing more trials. If the money and confidence in the model are available, more samples of the repository system model should be taken. The extrapolation uncertainty then becomes less extreme, and the two curves converge.

FIG. 22. Comparison of the extrapolated best-fit curve and curve that includes the tail-extrapolation uncertainties.

6.0 EPILOGUE

A method has been devised to incorporate today's technical uncertainties in a numerical simulation of a repository's performance. The intent of this method is to develop a unified probabilistic approach, through making appropriate compromises with mathematical rigor, to obtain a recognizable, scientific result predicting repository performance.

The first concern with such a scheme, which cannot be overcome in a rigorous fashion, is the handling of tails of distributions. Scientific judgment, not rigor, will be required to establish low-probability tails. We handle this using two techniques. First, the low-probability tails are handled for descriptive parameters by allowing the scientist to specify realistic ranges of the distribution function. The normalization of the function is over the range chosen. Second, the dose-curve tails are obtained by extrapolating with a suitably chosen function to low-probability outcomes.

A second concern is that the hypothetical model in the scientific method is always judgmental. It is experience with the model and robustness of the results with respect to model choices which provide high confidence predictions.

A third concern is that unforeseen processes are not included in a simulation. It is only through scientific experience and dialogue that such processes are discovered and incorporated.

The above concerns are inherent limitations on our ability to predict the future. Any scheme must deal with these. In our scheme we specify actions to handle them. Hopefully, the scheme will provide the reader with useful ideas on how to bridge the gaps between physical reality, predictive uncertainties, and institutional concerns.

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