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Constructing Probability Distributions of Uncertain Variables in Models of the Performance of the Waste Isolation Pilot Plant: The 1990 Performance Simulations

Martin S. Tierney

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Sandia National Laboratories
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CONSTRUCTING PROBABILITY DISTRIBUTIONS OF UNCERTAIN VARIABLES IN MODELS OF THE PERFORMANCE OF THE WASTE ISOLATION PILOT PLANT: THE 1990 PERFORMANCE SIMULATIONS

Martin S. Tierney
Safety and Reliability Analysis Division
Sandia National Laboratories
Albuquerque, New Mexico

ABSTRACT

A five-step procedure was used in the 1990 performance simulations to construct probability distributions of the uncertain variables appearing in the mathematical models used to simulate the Waste Isolation Pilot Plant's (WIPP's) performance. This procedure provides a consistent approach to the construction of probability distributions in cases where empirical data concerning a variable are sparse or absent and minimizes the amount of spurious information that is often introduced into a distribution by assumptions of nonspecialists. The procedure gives first priority to the professional judgment of subject-matter experts and emphasizes the use of site-specific empirical data for the construction of the probability distributions when such data are available. In the absence of sufficient empirical data, the procedure employs the Maximum Entropy Formalism and the subject-matter experts' subjective estimates of the parameters of the distribution to construct a distribution that can be used in a performance simulation.

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CONTENTS

FIGURES

Figure

TABLES

Table

EXECUTIVE SUMMARY

A five-step procedure was used in the 1990 performance simulations to construct probability distributions of the uncertain variables appearing in the mathematical models used to simulate the Waste Isolation Pilot Plant's (WIPP's) performance. Figure E-1 summarizes the steps in the procedure.

This procedure provides a consistent approach to the construction of probability distributions in cases where empirical data concerning a variable are sparse or absent and minimizes the amount of spurious information that is often introduced into a distribution by assumptions of nonspecialists. The procedure gives first priority to the professional judgment of subject-matter experts and emphasizes the use of site-specific empirical data for the construction of the probability distributions when such data are available. In the absence of sufficient empirical data, the procedure employs the Maximum Entropy Formalism and the subject-matter experts' subjective estimates of the parameters of the distribution to construct a distribution that can be used in a performance simulation.

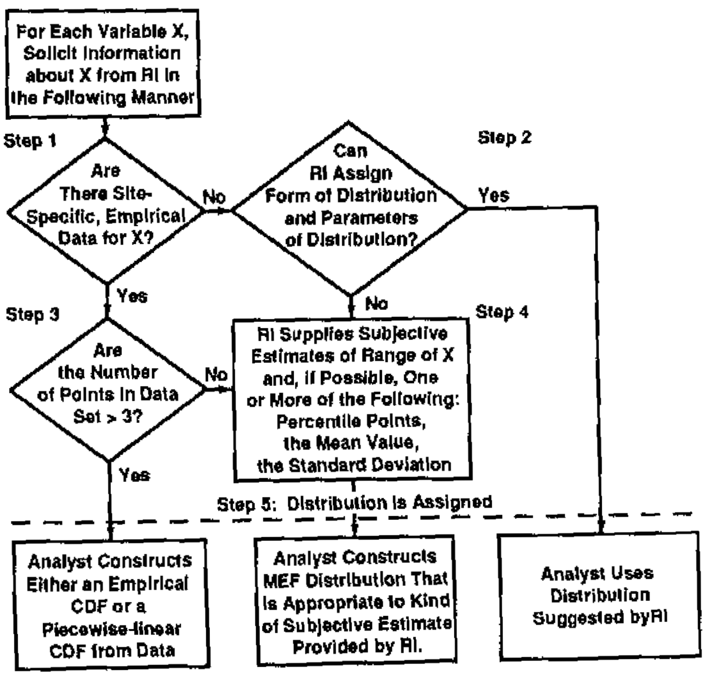

Figure E-1. The Five-Step Procedure Used to Construct Cumulative Distribution Functions (CDFs) for the 1990 Performance Simulations. RI refers to responsible investigator (i.e., subject-matter expert); MEF refers to the Maximum Entropy Formalism.

I. INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) is a research and development facility authorized by Congress (Public Law 96-164 [1980]) for the purpose of demonstrating the safe management, storage, and eventual disposal of those defense-generated transuranic (TRU) wastes that the U.S. Department of Energy (DOE) may designate as requiring deep geologic disposal. The DOE has established a program (hereinafter called the WIPP Project) to conduct the scientific and engineering investigations that are necessary for the demonstrations authorized by Congress. Further background on the WIPP and the WIPP Project can be found in U.S. DOE (1980) and U.S. DOE (1990).

The DOE will dispose of designated TRU wastes at the WIPP repository only after demonstrating compliance with the requirements of the U.S. Environmental Protection Agency's (EPA's) *Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes; Final Rule, 40 CFR Part 191*, (the Standard, EPA, 1985). The part of the Standard most relevant to this report, Subpart B or the "Environmental Standards for Disposal," sets qualitative and numerical requirements on the postclosure performance of the WIPP. (Although Subpart B of the Standard was remanded to the EPA by the United States Court of Appeals for the First Circuit, the WIPP Project will continue to respond to the Standard as first promulgated until a new Standard is in place [U.S. DOE and State of New Mexico, 1981].) In particular, the "Containment Requirements" in § 191.13 of Subpart B set numerical limits on the likelihoods that cumulative releases of radioactivity from the WIPP System to the accessible environment, for 10,000 years after closure of the system, will exceed certain prescribed levels. Demonstrating compliance with the Standard is the same as establishing a reasonable assurance that the numerical limits on the likelihoods of the prescribed levels of release specified in the Containment Requirements will not be exceeded. Further background on the Containment Requirements can be found in the Standard and in Tierney (in prep.).

In addition to specifying numerical limits, the Containment Requirements also suggest a general approach to the testing of compliance with the numerical limits on the likelihoods of cumulative releases of radioactivity from the disposal system. The EPA calls this general approach "performance assessment" and suggests that, if practicable, its end-product should be an overall probability distribution of cumulative releases of radioactivity to the accessible environment. The published guidance for interpreting and implementing the Containment Requirements suggests that the overall probability distribution should take the form of a "... 'complementary cumulative distribution function' that indicates the probability of exceeding various levels of release" (EPA, 1985, Appendix B). In practice, estimators of such complementary cumulative distribution functions (CCDFs) are constructed by Monte Carlo simulations of the behavior of the total system during its period of performance. Background on the uses of Monte Carlo simulation in performance assessment can be found in Tierney (in prep.).

Monte Carlo simulations of the WIPP System require three things: (1) a suite of mathematical models (usually implemented on a computer) that can predict the amount of radioactivity released from the WIPP System when it is subject to the geologic, anthropogenic, and climatic conditions that could prevail during the period of performance; (2) an identification of the independent variables that appear in the mathematical models; and (3) the assignment of probability distributions to the sensitive independent variables in a manner that reflects the state of knowledge about the likelihood of the actual values these variables may have in the real system (Tierney, in prep.). Background on the models used in the WIPP simulations can be found in Lappin et al. (1989), Marietta et al. (1989), Rechard et al. (1990a) and other documents cited in these reports. Background on sensitivity studies of selected variables of WIPP-system models can be found in Rechard et al. (1990a). The present report is concerned with the procedures that were used in 1990 to provide item 3, an assignment of probability distributions to the important independent variables of the WIPP performance models.

Purpose of This Report

The WIPP Project has performed preliminary simulations of the WIPP System with the purpose of demonstrating the applicability of the methods and models it has developed for testing compliance with the Containment Requirements (Marietta et al., 1989). Rechard et al. (1990a, Appendix A) listed the approximately 240 distinct independent variables that could appear in the mathematical or computer-based models used in these simulations. Most of these variables specify the physical, chemical, or hydrologic properties of the rock formations in which the WIPP is placed; a substantial number of the variables specify physical or chemical properties of engineered materials and the waste form; some are the dimensions of engineered features of the facility, and some pertain to future climatic variability or future episodes of exploratory drilling at the WIPP. About 60 of the 240 variables are judged to warrant uncertainty analysis; preliminary ranges of variability are given for these variables in Appendix A of Rechard et al. (1990a).

Preliminary simulations of WIPP performance (Marietta et al., 1989) included up to 40 of the approximately 60 uncertain variables in the Latin hypercube sampling (LHS) scheme currently being used by the WIPP Project in its Compliance Assessment Methodology Controller (CAMCON, see Rechard et al., 1989). Background on the assignment of probability density functions (PDFs) to these variables can be found in Appendix C of Marietta et al. (1989). No systematic procedures were used to assign PDFs to these variables: the distributions were assigned by WIPP analysts largely on the basis of limited data from Lappin et al. (1989), data from analogous (non-WIPP context) situations described in the literature and, in a few instances, on the basis of the professional judgment of subject-matter experts. Because the simulations of Marietta et al. (1989) were primarily made for demonstrational purposes, the lack of defensible and systematic procedures for the assignment of probabilities in these studies was not a serious flaw. Subsequent review of this work clarified the need for such procedures in future simulations that would be used to test compliance with the Containment Requirements.

The present, brief report describes and rationalizes the systematic procedure that was used in 1990 by the WIPP Project to construct probability distributions (cumulative distribution functions [CDFs] or probability density functions [PDFs]) for the uncertain independent variables in the WIPP performance models. The procedure is described and applied to variables currently being sampled in the WIPP performance models in Chapter II. Technical details of the procedure are also provided in Chapter II.

The 1990 procedure is described in this report to elicit reviewer's comments and start the review cycle. The WIPP Project has been asked to perform iterative performance assessments semiannually, with annual documentation of these assessments. A widely acceptable final compliance assessment depends on constructive feedback from peer reviewers of each annual assessment. This brief report is intended to focus some of the review efforts on a critical component of the performance-assessment process: construction of CDFs or PDFs.

Issues Not Addressed in This Report

Owing to limited information and time constraints, it has not been possible to address all the issues that are normally associated with the construction of probability distributions for a set of model variables. Important issues not treated or only mentioned here are

(a) The effects of possible dependencies among the different kinds of model variables on the assignment of probability distributions to those variables;

(b) The role of spatial correlations in constructing probability distributions for the variables of a lumped-parameter model;

(c) The assignment of extreme-value probabilities to a variable on the basis of a limited number of observations of the variable;

(d) The assignment of numerical probabilities to parameters of natural and anthropogenic phenomena that may occur in the far future.

Because of the lack of information, WIPP Project analysts have assumed that all of the approximately 60 uncertain variables in their mathematical models are independent (though not identically distributed) random variables. With one exception (the lumped parameters specifying WIPP room hydraulic conductivities and porosities), the possible effects of spatial correlations on reducing the variances of the variables in certain lumped-parameter performance models have been ignored. Owing to limited data, the extreme-value probabilities of most of the sensitive variables cannot be estimated with great confidence. Finally, the problem of assigning probabilities to the parameters of processes and events that may occur at the WIPP in the far future is only beginning to be addressed. The demonstrational performance simulations (Marietta et al., 1989) considered scenarios for climatic change and human intrusion at the WIPP in which the climatic and intrusion parameters were assigned fixed values. Current performance simulations have attempted to introduce uncertainty in these parameters in the simplest possible ways. For the parameters of the human-intrusion scenarios, see Appendix C of Tierney (in prep.).

The fact that issues (a) and (b) were not addressed in the 1990 performance simulations severely limits the validity of some of the CDFs that were constructed by the procedure described in this report; further discussion of these issues is provided in Chapter III.

II. PROCEDURES FOR CONSTRUCTING PROBABILITY DISTRIBUTIONS

An Outline of the Procedures

In 1990, the WIPP Project constructed probability distributions for the uncertain variables appearing in performance models of the WIPP System by following steps 1 through 5 described below. Explanations of the meaning of underlined terms appearing in descriptions of the steps are deferred until later sections of this chapter. The acronym RI, "responsible investigator," will hereinafter mean the Sandia National Laboratory investigator who is judged to be the expert in the subject matter of the variable.

STEP 1

Determine the existence of site-specific empirical data for the variable in question; i.e., find a documented set of site-specific sample values of the variable. If empirical data sets exist, go to Step 3; if no empirical data sets are found, go to Step 2.

STEP 2

Request that the RIs supply a specific shape (e.g., normal, lognormal, etc.) and associated numerical parameters for the distribution of the variable. If the RIs assign a specific shape and numerical parameters, go to Step 5; if the RIs cannot assign a specific shape, go to Step 4.

STEP 3

Determine the size of the combined empirical data sets. If the number of values in the combined data set is >3, use the combined data to construct an empirical cumulative distribution function or, alternatively, a piecewise-linear cumulative distribution function, and then go to Step 5. If the number of variables in the combined data set is ≤3, go to Step 4.

STEP 4

Request that the RIs provide subjective estimates of (a) the range of the variable (i.e., the minimum and maximum values taken by the variable) and (b) if possible, one of the following (in decreasing order of preference): (1) percentile points for the distribution of the variable (e.g., the 25th, 50th, and 75th percentiles), (2) the mean value and standard deviation of the distribution, or (3) the mean value. Then, as justified by the Maximum

Entropy Formalism (MEF), construct one of the following distributions depending upon the kind of subjective estimate that has been provided and go to Step 5.

A uniform distribution (PDF) over the range of the variable.

A piecewise-linear CDF based on the subjective percentiles.

A truncated normal distribution based on the subjective range, mean value, and standard deviation.

A truncated exponential distribution based on the subjective range and mean value.

STEP 5

End of procedures; distribution is assigned.

This five-step procedure was motivated by a desire to maintain as close a connection between situation-specific data/information and model parameters as possible. Though obviously not unique, the formulation of the procedure was guided by two axioms: (1) a probability distribution describing a variable should, to the maximum extent practicable, be constructed from empirical data and information that are site specific, and (2) if numerical data (i.e., sample values for the quantity) are few or nonexistent, probability distributions for that quantity should be constructed using *only* those subjective but quantified judgments about the quantity that are made by experts in the subject matter pertaining to the quantity. It is assumed that a subject-matter expert will take account of all relevant information, site-specific or generic, in making subjective but quantified judgements about the shape of a variable's distribution.

Axiom 1 recognizes that empirical, system-specific data — combined with proven theoretical concepts and informed, professional interpretation of the data — are the only link between the real system and the mathematical models that are being used to study the real system's behavior. The need for Axiom 2 arises when, for various reasons, numerical data for an independent variable of a model are few or entirely absent (unfortunately, this is the situation for the majority of the uncertain independent variables in current WIPP performance models). When data are lacking, professional judgment is all that is left; Axiom 2 ensures that only subjective information provided by persons with specialized knowledge of the variable (usually, persons other than the performance-assessment analyst) will be included in determining the form of the probability distribution. Adherence to Axiom 2 practically dictates the use of a particular method called the Maximum Entropy Formalism (MEF, see below) for constructing probability distributions from quantifiable subjective judgments.

Empirical Cumulative Distribution Functions

Suppose that one is given $N > 3$ sample values of an uncertain independent variable X that appears in a WIPP performance model,

$$X_1,\ X_2,\ X_3,\ \ldots,\ X_N\ .$$

In the remainder of this chapter, it is assumed that the X_ns are independent, identically distributed random variables with a common (but unknown) CDF that is here denoted by F(x). Furthermore, since all of the WIPP performance-model variables are positive, it will be assumed that X is a non-negative variable; i.e., $X \geq 0$. (The reader should nevertheless keep in mind the ways the assumption of independence could fail, e.g., the possibility of a biased sample arising from intervariable and spatial correlations among different kinds of variables.)

Upon ordering the sample data, one gets

$$X_1^*,\ X_2^*,\ X_3^*,\ \ldots,\ X_N^*,\quad \text{with } X_n^* \leq X_{n+1}^*\ ,\ n = 1,\ 2,\ 3,\ \ldots,\ N\text{-}1\ .$$

If X is an intrinsically discrete variable, or if X is intrinsically continuous and some of the X_n^*s are identical (perhaps owing to the precision with which the original X_ns were measured), the ordered sample data can be grouped into $M \leq N$ ordered pairs,

$$(x_1,f_1),\ (x_2,f_2),\ (x_3,f_3),\ \ldots,\ (x_M,f_M)\ ,$$

where $(x_1, x_2, \ldots x_M)$ is the ordered set of distinct values among the X_ns and the f_ms denote the multiplicities of the X_ms. For example, if X_6 appears three times in the data set, then $f_6 = 3$. Clearly, $1 \leq f_m < N$, and

$$\sum_{m=1}^{M} f_m = N\ .$$

As an example, one can take the 15 sample values of Culebra tortuosity cited in Table E-9 of Lappin et al. (1989); these values become the 12 ordered pairs: (0.03,1), (0.04,1), (0.08,1), (0.09,3), (0.10,1), (0.12,1), (0.13,1), (0.14,1), (0.16,1), (0.21,2), (0.29,1), (0.33,1).

The <u>empirical percentiles</u> p_m associated with the sample data are defined as the ratio of the number of values in the set $\{X_n, 1 \le n \le N\}$ that are less than or equal to x_m, $1 \le m \le M$, to the total number of values in the set (= N). Using this definition, it follows that

$$p_{m+1} = p_m + (1/N)f_{m+1}, \quad p_1 = f_1/N \text{ ; and so}$$

$$p_m = (1/N) \sum_{i=1}^{m} f_i, \; 1 \le m \le M .$$

The p_ms are a nondecreasing sequence of numbers ≤ 1 with $p_M = 1$.

The <u>empirical cumulative distribution function</u> (empirical CDF) associated with the sample data $X_1, X_2, \ldots, X_N$ is the piecewise constant function here denoted by $F_c(\xi)$ and defined for $\xi \, \varepsilon \, [0,\infty)$ by

$$F_c(\xi) = \begin{cases} 0 & \text{if } \xi \le x_1 , \\ P_m & \text{if } x_m < \xi \le x_{m+1} , \; m = 1,2, \ldots, M-1, \\ 1 & \text{if } \xi > x_M . \end{cases}$$

The empirical CDF associated with the 15 sample values of tortuosity from Table E-9 of Lappin et al. (1989) is drawn as the dotted curve on Figure II-1.

The empirical CDF $F_c(\xi)$ is an <u>unbiased estimator</u> (see Blom, 1989, p. 194) of the unknown distribution of the variable X (Blom, 1989, p. 216).

The <u>mean value</u> or <u>expected value</u> of the variable X with respect to the empirical CDF $F_c(\xi)$ is here denoted by $\langle X \rangle_c$ and is the same as the usual sample mean, that is,

$$\langle X \rangle_c = (1/N) \sum_{m=1}^{M} f_m x_m \; ;$$

hence $\langle X \rangle_c$ is an unbiased estimator of the expected value of the unknown distribution F(x). The expected value associated with the empirical CDF for tortuosity in Figure II-1 is 0.14.

The <u>variance</u> of the variable X with respect to the empirical CDF $F_c(\xi)$ is here denoted by s_c^2 and can be computed as follows:

$$s_c^2 = (1/N) \sum_{m=1}^{M} f_m [x_m - \langle X \rangle_c]^2 .$$

This is not an unbiased estimator of the variance of X, but the quantity $[N/(N-1)]s_c^2$ (the usual sample variance) is an unbiased estimator. The s_c^2 associated with the empirical CDF for the tortuosity data in Figure II-1 is 6.9×10^{-4} (hence the standard deviation $s_c \approx 0.083$).

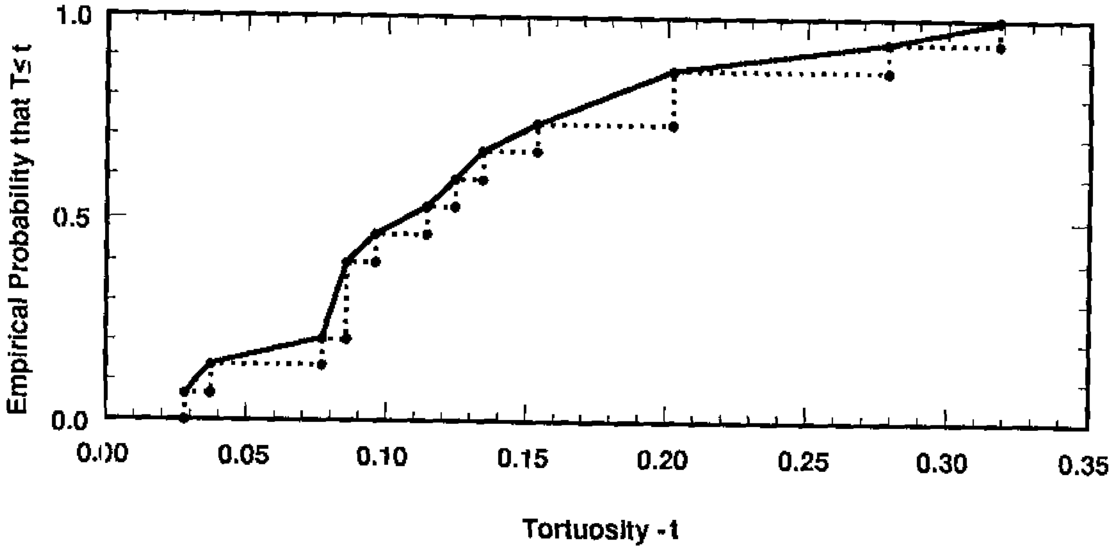

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Figure II-1. Empirical and Piecewise-Linear CDFs for Tortuosity Data. Dotted line is empirical CDF; solid line is Piecewise-Linear CDF.

Piecewise-Linear Cumulative Distribution Functions

Use of an empirical CDF in practical Monte Carlo calculations may have some drawbacks. All of the sampling techniques used in Monte Carlo simulation (e.g., random sampling, LHS) require the drawing of a number of random variates from each of the distribution functions for uncertain model variables. Inspection of the example empirical CDF shown in Figure II-1 reveals that drawing random variates from an empirical CDF will only give back the discrete data points $x_1, x_2, \ldots, x_M$ with respective frequencies f_1/N, f_2/N, ..., f_M/N as $N \to \infty$. Of course, this is the intended result when the variable X is an intrinsically discrete random variable (e.g., $X_n = n$ could be the number of times an event occurs in a fixed period of time). But if the variable X is an intrinsically continuous variable (e.g., the spatial average of tortuosity or porosity) and the points of the empirical data set $\{X_n, 1 \le n \le N\}$ are few and sparsely placed on the real line, it is possible that the sampled variates used in the simulations will always "miss" one or more of those critical values of X at which the output of the performance model could be particularly sensitive. For this reason, performance-assessment analysts prefer to sample from continuous CDFs for those variables that are known to be continuously distributed.

The empirical CDF described above can be modified and cast into a continuous distribution in several ways. Perhaps the simplest way is to draw straight lines between the vertices of the empirical CDF, i.e., the points (0,0), (x_1,p_1), (x_2,p_2), ..., (x_M,p_M) on the graph of the CDF (for example, see the solid lines so drawn on Figure II-1 for the tortuosity data). The <u>piecewise-linear CDF</u> constructed in this way is here denoted by $F_\ell(\xi)$ and is analytically expressed by

$$F_\ell(\xi) = \begin{cases} 0 & \text{if } \xi \le 0, \\ P_{m-1} + \dfrac{f_m(\xi - x_{m-1})}{N(x_m - x_{m-1})} & \text{if } x_{m-1} < \xi \le x_m,\ m = 1, 2, \ldots, M, \\ 1 & \text{if } \xi > x_M, \end{cases}$$

where $p_0 = 0$ and $x_0 = 0$.

Inspection of the example shown on Figure II-1 reveals that drawing random variates from a piecewise-linear CDF will give back a random selection of all of the values of the variable X that lie between 0 and x_M, not just the original values x_1, x_2,...,x_M. The author has not found or been able to develop a proof that a piecewise-linear CDF constructed in this way is an unbiased estimator of the unknown distribution of the variable X.

The mean value or expected value of the CDF $F_\ell(\xi)$ is here denoted by $\langle X\rangle_\ell$ and can be expressed as

$$\langle X\rangle_\ell = (1/N)\sum_{m=1}^{M} f_m(x_m + x_{m-1})/2 \quad .$$

The variance of the CDF $F_\ell(\xi)$ is denoted by s_ℓ^2 and can be expressed as

$$s_\ell^2 = (1/N)\sum_{m=1}^{M} f_m(x_m^2 + x_m x_{m-1} + x_{m-1}^2)/3 - \langle X\rangle_\ell^2 \ .$$

The author has not found or been able to develop a proof that $\langle X\rangle_\ell$ and s_ℓ^2 are unbiased estimators of the respective mean and variance of the unknown distribution F(x). For the CDF for the tortuosity data shown on Figure II-1, $\langle X\rangle_\ell = 0.13$ and $s_\ell^2 = 5.0 \times 10^{-2}$.

It is somewhat surprising that the piecewise-linear CDF obtained by simply drawing straight lines between empirical-percentile points of an empirical CDF is the same distribution that is obtained by using the Maximum Entropy Formalism (MEF; to be discussed in the next section) and constraints specified by empirical percentile points.

The Maximum Entropy Formalism

The literature on the Maximum Entropy Formalism (MEF) is now vast; the reader should consult the reviews edited by Levine and Tribus (1978), or the recent monograph by Jumarie (1990), for thorough discussions of the foundations and areas of application of this subject. The MEF has been used before to construct prior probability distributions of uncertain variables in nuclear-risk assessment models: See Cook and Unwin (1986) and Unwin et al. (1989).

In this report, the MEF is simply regarded as a consistent mathematical procedure for the derivation of a probability distribution function for an uncertain variable, X, from a set of quantitative constraints on the form of that distribution; e.g., quantitative statements about the range, the mean, the variance, or the percentiles of the distribution. The quantitative constraints may be empirical constraints, i.e. constraints based on sample values of the variable, or subjective constraints based on professional judgment.

The central problem of the MEF is the determination of extrema of the so-called <u>entropy functional</u>, defined by

$$S(f) = -\int_a^b f(x)\ell n[f(x)]dx,$$

over the set of all probability density functions, f(x), which are nonzero in the range [a,b] and which satisfy prescribed, quantitative constraints.

The entropy functional is the continuous version of the information-theoretic entropy

$$S = -k\sum_i P_i \ \ell n \ P_i \ ,$$

i.e., it is the expected value of Shannon's measure,

$$I(X_i) = -k \ \ell n \ P_i, \ k \text{ a constant} \ ,$$

of the amount of information gained by observing the outcome of an experiment in which a random variable X_i is observed to take on the value x_i with probability P_i (Hamming 1991; Ch. 7). The entropy functional has also been interpreted as a measure of the amount of uncertainty inherent in a PDF or as a measure of the amount of information that would be required to specify completely the value of a random variable X (for the idea that entropy is "missing" information, see Baierlein, 1971). Thus, finding an extremum of the entropy functional subject to prescribed constraints can be construed as finding the PDF, within the set of all PDFs that incorporate the information inherent in the constraints, which maximizes the amount of remaining information that must be supplied in order to completely specify the value of the uncertain variable X. Use of the MEF can minimize the amount of spurious information that often enters into the construction of a PDF from sparse data or limited quantitative information.

The prescribed informational constraints are best expressed as integral constraints, i.e., they should take the form

$$\int_a^b g_m(x)f(x)dx = C_m, \quad m = 0, 1, 2, \ldots, M ,$$

where the g_ms are given, integrable functions of x on the interval [a,b] and the C_ms are given constants. One necessary constraint on a PDF is that its integral over [a,b] must equal one; thus one conventionally takes $g_0 = 1$ and $C_0 = 1$. By expressing the constraints in this way, one can derive a general solution to the problem (in the calculus of variations) of maximizing S(f) subject to the M+1 constraints (see, for example, Tribus, 1969). The maximizing PDF, here denoted by $f^*(x)$, is given by

$$f^*(x) = Z^{-1}(\lambda_1, \lambda_2, \ldots, \lambda_M)\exp\left[- \sum_{m=1}^{M} \lambda_m g_m(x) \right] ,$$

where Z^{-1} is the reciprocal of Z and

$$Z(\lambda_1, \lambda_2, \ldots, \lambda_M) = \int_a^b \exp\left[- \sum_{m=1}^{M} \lambda_m g_m(x) \right] dx .$$

The λ_m, $1 \le m \le M$, are constants (Lagrange multipliers) to be determined by solving the following set of M equations in M unknowns:

$$-(\partial/\partial\lambda_m)\ell nZ = C_m, \quad 1 \le m \le M .$$

The special forms of $f^*(x)$ that arise from this formalism when the constraints mentioned in the outline of the five-step procedure are applied are of particular interest:

a. When only the range of X is given (i.e., no constraints other than normalization of the PDF), then $f^*(x)$ is the uniform distribution on the interval [a,b]. Obviously, this makes sense only if $|b-a| < \infty$, i.e, the range of the variable X is bounded.

b. When the range and M percentile points of the CDF are given, then $f^*(x)$ is a weighted sum of M uniform distributions that vanishes outside the range [a,b] and the associated CDF is piecewise linear. In this case, the $M \geq 1$ constraints are of the form

$$g_m(x) = u(x_m - x), \quad C_m = p_m, \; m = 1, 2, 3, \ldots, M ,$$

where u(•) is the unit step function (Abramowitz and Stegun, 1964, p. 1020, 29.1.3), the x_ms are given percentile points in the interval [a,b], and the p_ms are the corresponding percentiles.

c. When the range, the mean value, and the variance (or coefficient of variation) of the variable X are given, then $f^*(x)$ is a truncated normal distribution that vanishes outside the interval [a,b]. In this case, the two constraints are of the form

$$g_1(x) = x, \; C_1 = \mu \; ; \; g_2 = (x - \mu)^2, \; C_2 = \sigma^2 ,$$

where μ and σ^2 are respectively the given mean value and variance.

d. When the range and only the mean value of the variable X are given, then $f^*(x)$ is a truncated exponential distribution that vanishes outside the interval [a,b]. In this case, $g_1 = x$ and $C_1 = \mu$.

Proofs of Cases a, c, and d can be found in Tribus (1969). The author has not been able to locate a proof of Case b and has therefore supplied his own proof below.

Let the empirical or subjective percentile points be the given as $M \geq 1$ ordered pairs (x_1,p_1), (x_2,p_2), ..., (x_M,p_M) with

$$0 \leq a < x_1 < x_2 < \ldots < x_M < b < \infty; \qquad p_1 < p_2 < \ldots < p_M$$

and $0 < p_m < 1$ for all $m > 0$. For convenience, define

$$x_0 = a, \ p_0 = 0; \quad x_{M+1} = b, \ p_{M+1} = 1 \ .$$

The constraints on the candidate PDFs, $f(x)$, may then be written as

$$\int_a^b u(x_m - s) f(s) ds = p_m, \ m = 0, 1, 2, \ldots, M+1 \ ,$$

where $u(")$ is the unit step function (Abramowitz and Stegun, 1964, p. 1020). The PDF that maximizes the entropy functional is therefore

$$f^*(x) = \exp\left[\sum_{m=1}^{M} \lambda_m u(x_m - x) - 1\right] \ ,$$

where the λ_ms are constants to be determined from the constraints. Inspection of this PDF shows that it is a piecewise-constant function on the interval $[a,b]$; i.e., $f^*(x) = A_m$, if $x_{m-1} < x \leq x_m$, with A_m a different constant for each $m = 1, 2, \ldots, M+1$. The constants A_m are simply related to the constants λ_m, and it is easier to determine the A_ms from the constraints. For example, consider the integral of $f^*(x)$ between x_{m-1} and x_m. This integral is $(x_m - x_{m-1})A_m$, but by the constraints it is also equal to $(p_m - p_{m-1})$. It follows that

$$A_m = (p_m - p_{m-1})/(x_m - x_{m-1}), \quad m = 1, 2, \ldots, M+1.$$

By integrating $f^*(x) = A_m$, $m = 1,2,\ldots,M+1$, between $x_0 = a$ and a point $\xi >$ a, one finds the CDF associated with $f^*(x)$:

$$F^*(\xi) = \begin{cases} 0 & \text{if } 0 < \xi \leq a, \\ p_{m-1} + (p_m - p_{m-1})(\xi - x_{m-1})/(x_m - x_{m-1}), & \text{if } x_{m-1} < \xi \leq x_m, \\ 1 & \text{if } \xi > b \ . \end{cases}$$

This result is a piecewise-linear CDF of the kind described earlier in this chapter.

Once again, the reader should take note that in using the MEF, the ranges, percentiles and percentile points, mean values, and variances to be supplied in Cases a through d can be either empirical or subjective numbers; that is, they can be numbers derived from measurements of the variable X, or they can be furnished as the "best estimates" of the RIs. Of course, if only subjective estimates are used to form the parameters of an MEF distribution, it is meaningless to inquire whether that distribution is an unbiased estimator of the unknown distribution, F(x). The resulting distribution is purely subjective and can only reflect the accuracy of the PIs' best estimates of the distribution's parameters.

An Application of the Procedures

The most recent simulations of WIPP performance used probability distributions obtained by the five-step procedure described above. The results of this first, informal trial of the procedure are summarized in Table II-1: column 1 of the table names the 29 variables that were sampled in the recent simulations and gives their physical units; column 2 names the kind of distribution that was ultimately assigned; and column 3 briefly states the source of information and the basis for the assignment of the distribution named in column 2.

In this first trial of the procedures, no formal elicitation of expert judgment of the type suggested by Bonano et al. (1990) was used. A memo was sent to WIPP Project RIs in Department 6340 of Sandia National Laboratories asking that they provide any information they might have concerning each of the 29 variables; the requested information was to be supplied in one or more of the following forms and listed in order of decreasing preference on the part of the performance-assessment analyst:

(1) A table of WIPP-specific, measured values of the variable.

(2) Reasoned estimates of percentile points for the variable; i.e. the provision of statements like "90 percent of solubility values for radionuclide species A lie below 10^{-4} molar."

(3) Reasoned estimates of the mean value and standard deviation of the variable.

(4) Reasoned estimates of only the mean value of the variable.

(5) At minimum, and always in addition to information of types 1 through 4, reasoned estimates of the maximum and minimum values (range) that the variable could assume in the context of the WIPP system.

In addition to a written request for information, informal meetings were held with the PIs in order to explain the purpose of the request for information and to help their understanding of some of the statistical terms used in the memorandum. These informal meetings revealed that some of the RIs were

TABLE II-1. PROBABILITY DISTRIBUTIONS FOR VARIABLES SAMPLED IN CURRENT WIPP PERFORMANCE SIMULATIONS*

Variable Name and Units	Type of Distribution	Source or Basis for Distribution†
1. Salado Capacitance (Pa^{-1})	Lognormal	Assigned by RI.
2. Salado Permeability (m^3)	Piecewise Linear	MEF-empirical percentiles from data provided by RI.
3. Salado Pressure (MPa)	Uniform	MEF-bound provided by RI.
4. Room-Waste Solubility (all radionuclide species, kg/kg)	Loguniform	Assigned by RI.
5. Room-Time of First Intrusion	Modified Exponential	Appendix C of Tierney (in prep.).
6. Brine Pocket Initial Pressure (MPa)	Piecewise Linear	MEF-bounds and median provided by RI.
7. Borehole Permeability m^2	Lognormal	Freeze and Cherry, 1979.
8. Borehole Porosity (dimensionless)	Normal	Freeze and Cherry, 1979.
9. Brine Pocket Bulk Volume (m^3)	Uniform	MEF-bounds provided by RI.
10. Culebra Tortuosity (dimensionless)	Piecewise Linear	MEF-empirical percentiles from data in Tables E-9 of Lappin et al., 1989.
11. Culebra Diffusion Coefficient (all radionuclide species, m^2/s)	Uniform	MEF-bounds are maximum and minimum of values given in Table A-8 of Rechard et al., 1990a.
12. Culebra Fracture Spacing (m)	Piecewise Linear	MEF-bounds and median provided by RI.

* A complete description of the probability distributions for all variables used in the 1990 performance simulations can be found in Rechard et al. (1990b).

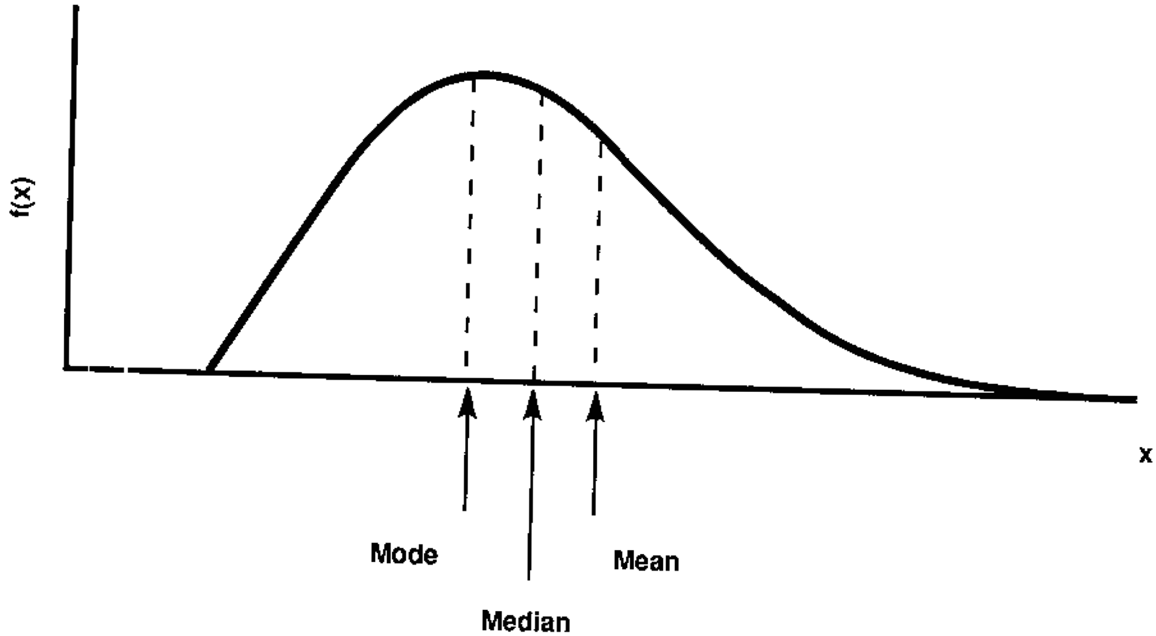
† The RIs' responses that provided the sources or basis for each distribution are documented in Memos 3-11 and Letters 1a and 1b of Appendix A of Rechard et al. (1990b).

TABLE II-1. PROBABILITY DISTRIBUTIONS FOR VARIABLES SAMPLED IN CURRENT WIPP PERFORMANCE SIMULATIONS (concluded)

Variable Name and Units	Type of Distribution	Source or Basis for Distribution
13. Culebra Recharge Factor (dimensionless)	Uniform	Marietta et al., in prep.
14. Culebra Precipitation Factor (dimensionless)	Uniform	Marietta et al., in prep.
15. Borehole cross-sectional area (m^2)	Empirical	Data provided by RI.
16-19. Culebra - Matrix Retardation Factors for Plutonium, Americium, Neptunium and Uranium (dimensionless)	Piecewise Linear	MEF-subjective percentiles (0, 25, 50, 75, 100) provided by RI.
20-23. Culebra - Fracture Retardation Factors for Plutonium, Americium, Neptunium and Uranium (dimensionless)	Piecewise Linear	MEF-subjective percentiles (0, 25, 50, 75, 100) provided by RI.
24-29. Culebra Hydraulic Conductivity for Zones 1-7 (m/s)	Piecewise Linear	MEF-empirical percentiles from data provided by RI.

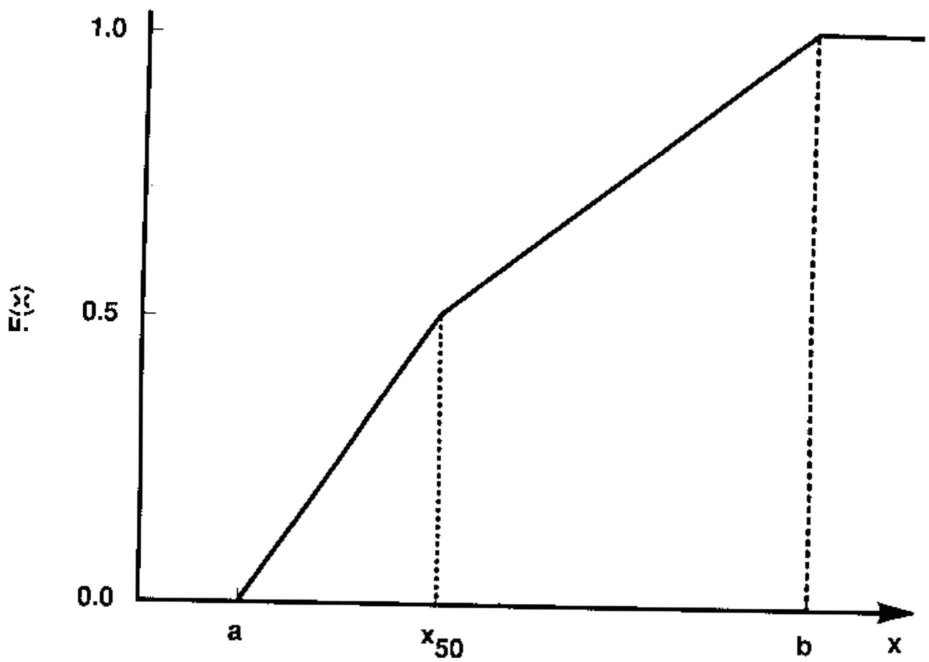
confused about the meanings of the several measures of the shape of a probability distribution (Figure II-2). In subsequent meetings, most of the RIs agreed that, in the absence of data, they could not supply reasoned estimates of the mean value, μ, or standard deviation, σ, of the unknown distribution and that the measures of location they had previously called "expected values" were more likely to be estimates of the median value, x_{50}, or the mode, x_{max}, of the distribution.

If the RI provided the range (a,b) and an estimate of the median, x_{50}, the MEF yielded the simple, piecewise-linear CDF illustrated in Figure II-3. Providing a subjective estimate of the mode of an unknown PDF was discouraged. In the absence of additional information about the value of the PDF at the mode (information usually not known to an RI), the use of a subjective mode as a constraint in the MEF only gives back the uniform distribution over the range (a,b), the same distribution that arises if the range alone is specified.



TRI-6342-580-0

3 Figure II-2. Typical PDF Showing the Different Measures of Location.



TRI-6342-667-0

5 Figure II-3. Piecewise-Linear CDF Based on Range and Median Value.

III. LIMITATIONS ON THE 1990 PROBABILITY DISTRIBUTIONS

The major limitations on the validity of the probability distributions constructed for the 1990 performance simulations are believed to be the consequence of two things:

(1) The effects of spatial averaging on the variance of model variables used in lumped-parameter models were ignored.

(2) Possible correlations between model variables were ignored.

The Effects of Spatial Averaging

Since most of the WIPP performance models are lumped-parameter models, many of the variables to be assigned CDFs in the WIPP performance models are actually spatial averages of physical quantities that can only be measured on spatial scales that are small compared with the spatial scale used in the models. For example, the effective hydraulic conductivity and porosity of a WIPP waste room (a structure having a volume of the order of 1000 m^3) are actually volumetric averages over the local hydraulic conductivity and porosity of approximately 1000 consolidated waste units (collapsed waste barrels) each having volumes of the order of one cubic meter. The RI usually provides information about variability of a quantity on the smaller of the two spatial scales. It is easy to show that use of this small-scale variability to reflect directly the variance in the lumped-parameter model variable will result in unnecessarily conservative CDFs. Very roughly, the following relationship holds between the variance of a volumetric average and the variance of the "local," small-scale quantity:

$$\sigma^2_{ave} \simeq (v/V)\sigma^2_{loc}$$

where v is a correlation volume and V is the volume over which the local physical quantity is to be averaged (analogous relationships hold for linear and areal averages). Although the precise size of the correlation volume is not known in every case, it is usually known that v << V. It follows that the variance of a volumetric average may be much smaller than the apparent variance of the local quantity. On the other hand, the mean value of the volumetric average should be equal to the mean value of the local quantity. The picture of the PDF for a spatial average that emerges from these remarks is one of a distribution that is sharply peaked about the mean value of the local quantity. In the absence of other kinds of information indicating uncertainty in the mean value of the local quantity, it would be inefficient to sample from such a highly peaked distribution; the variable in question would simply be assigned the best estimate of the mean value of the local quantity.

Thus, in seeking more information about those model variables that are known to be spatial averages of local quantities, it may be necessary to ask that experts provide scales of measurements and correlation lengths, and state their estimate of the uncertainty in the mean value of the local quantity, in addition to providing the observed or perceived variability of the local quantity itself.

Correlations Between Model Variables

All of the uncertain variables studied during the 1990 performance simulations were assumed to be independent random variables, although it was known in advance that many of them were interdependent, i.e. correlated in some way. Correlations of the model variables may arise from the fact that there are natural correlations between the local quantities used to determine the form of the model variable (e.g., local porosity could be strongly correlated with local permeability); or correlations of model variables may be implicit in the form of the mathematical model in which they are used. As an example of the latter circumstance, the current model for predicting WIPP-room hydraulic conductivity and porosity (see Rechard 1990b, Chapter III) makes these variables depend upon the volume fractions of specific waste forms (i.e., fractions of combustibles, metallics, sludges, etc.) contained in the entire waste inventory. These volume fractions are obviously uncertain variables themselves even though they were not treated as variables in the 1990 performance simulations. Taking account of the uncertainty in volume fractions would change estimates of the uncertainty in the mean value of the WIPP-room hydraulic conductivity and porosity.

Correlations among the important variables of the WIPP performance models need to be examined in detail since these model-dependent correlations may either increase or decrease the variance of a particular variable, and therefore effectively change the shape of that variable's CDF.

Distribution

FEDERAL AGENCIES

U. S. Department of Energy (6)
Office of Environmental Restoration
and Waste Management
Attn: Leo P. Duffy, EM-1
Jill E. Lytle, EM-30
Mark Duff, EM-34
Steve Schneider, EM-34
Clyde Frank, EM-50
Lynn Tyler, EM-50
Washington, DC 20585

U.S. Department of Energy (5)
WIPP Task Force
Attn: Mark Frei
G. H. Daly
Sandi Fucigna
12800 Middlebrook Rd.
Suite 400
Germantown, MD 29874

U.S. Department of Energy (5)
Office of Environment, Safety and
Health
Attn: Raymond P. Berube, EH-20
John Tseng, EH-20
Carol Borgstrum, EH-25
Ray Pelletier, EH-231
Kathleen Taimi, EH-232
Washington, DC 20585

U. S. Department of Energy (8)
Albuquerque Operations Office
Attn: Bruce G. Twining
J. E. Bickel
R. Marquez
K. A. Griffith
M. Wilson
D. Krenz
G. Runkle
C. Soden
P.O. Box 5400
Albuquerque, NM 87185-5400

U. S. Department of Energy (10)
WIPP Project Office (Carlsbad)
Attn: A. Hunt (4)
M. McFadden
V. Daub (4)
K. Hunter
P.O. Box 3090
Carlsbad, NM 88221-3090

U. S. Department of Energy, (5)
Office of Civilian Radioactive Waste
Management
Attn: Deputy Director, RW-2
Associate Director, RW-10
Office of Program
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Resources Management
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Attn: Director
P.O. Box E
Oak Ridge, TN 37831

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825 Jadwin Ave.
P.O. Box 500
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2753 S. Highland Drive
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Golden, CO 80402-0928

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P.O. Box 66
Miamisburg, OH 45343-0066

U.S. Department of Energy
Attn: Edward Young
Room E-178
GAO/RCED/GTN
Washington, DC 20545

U.S. Department of Energy
Advisory Committee on Nuclear
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Washington, DC 20585

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Programs (ANR-460)
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Washington, D.C. 20460

U.S. Nuclear Regulatory Commission
(4)
Division of Waste Management
Attn: Joseph Bunting, HLEN 4H3 OWFN
Ron Ballard, HLGP 4H3 OWFN
Jacob Philip, WMB
NRC Library
Mail Stop 623SS
Washington, DC 20555

U.S. Nuclear Regulatory Commission
(4)
Advisory Committee on Nuclear Waste
Attn: Dade Moeller
Martin J. Steindler
Paul W. Pomeroy
William J. Hinze
7920 Norfolk Avenue
Bethesda, MD 20814

Defense Nuclear Facilities Safety
Board
Attn: Dermot Winters
600 E. Street NW
Suite 675
Washington, DC 20004

Nuclear Waste Technical Review Board (2)
Attn: Don U. Deere
1111 18th Street NW #801
Washington, DC 20006

Neile Miller
Energy and Science Division
Office of Management and Budget
725 17th Street NW
Washington, DC 20503

U.S. Geological Survey
Branch of Regional Geology
Attn: R. Snyder
MS913, Box 25046
Denver Federal Center
Denver, CO 80225

U.S. Geological Survey
Conservation Division
Attn: W. Melton
P.O. Box 1857
Roswell, NM 88201

U.S. Geological Survey (2)
Water Resources Division
Attn: Cathy Peters
Suite 200
4501 Indian School, NE
Albuquerque, NM 87110

STATE AGENCIES

Bureau of Land Management
101 E. Mermod
Carlsbad, NM 88220

Bureau of Land Management
New Mexico State Office
P.O. Box 1449
Santa Fe, NM 87507

Environmental Evaluation Group (5)
Attn: Robert Neill
Suite F-2
7007 Wyoming Blvd., N.E.
Albuquerque, NM 87109

New Mexico Bureau of Mines and Mineral Resources (2)
Attn: F. E. Kottlowski, Director
J. Hawley
Socorro, NM 87801

NM Department of Energy & Minerals
Attn: Kasey LaPlante, Librarian
P.O. Box 2770
Santa Fe, NM 87501

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Mayor, City of Carlsbad
P.O. Box 1569
Carlsbad, NM 88221

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Executive Director
Carlsbad Department of Development
P.O. Box 1090
Carlsbad, NM 88221

Robert M. Hawk (2)
Chairman, Hazardous and Radioactive Materials Committee
Room 334
State Capitol
Sante Fe, NM 87503

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Deputy Director
New Mexico Environmental Improvement Division
P.O. Box 968
1190 St. Francis Drive
Santa Fe, NM 87503-0968

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New Mexico Waste Resources Research Institute
Box 3167
Las Cruces, NM 88001

Robert Bishop
Nuclear Management Resources Council
1776 I Street, NW
Suite 300
Washington, DC 20006-2496

Arthur Kubo
BDM Corporation
7915 Jones Branch Drive
McLean, VA 22102

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Slosky & Associates
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1675 Broadway
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Water Resources Division
U.S. Geological Survey (M/S 439)
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Menlo Park, CA 94025

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Palo Alto, CA 94303

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Gainesville, FL 32601

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200 Yale, NE
Albuquerque, NM 87131

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2260 University Drive
Newport Beach, CA 92660

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U.S. Geological Survey
431 National Center
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505 Valley Hill Drive
Atlanta, GA 30350

Christopher Whipple
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160 Spear St., Ste. 1380
San Francisco, CA 94105-1535

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Dr. Geraldine J. Grube
2101 Constitution Avenue
Washington, DC 20418

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583 Henderson Hall
University of Washington
Seattle, WA 98195

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Department of Nuclear Engineering
4153 Etcheverry Hall
University of California
Berkeley, CA 94720

Thomas A. Cotton
JK Research Associates, Inc.
4429 Butterworth Place, NW
Washington, DC 20016

Robert J. Budnitz
President, Future Resources
Associates, Inc.
2000 Center Street
Suite 418
Berkeley, CA 94704

C. John Mann
Department of Geology
245 Natural History Bldg.
1301 West Green Street
University of Illinois
Urbana, IL 61801

Frank W. Schwartz
Department of Geology and Mineralogy
Ohio State University
Scott Hall
1090 Carmack Rd.
Columbus, OH 43210

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Washington, DC 20036

Norman Rosenberg
Resources for the Future
1616 P St., NW
Washington, DC 20036

Max Singer
The Potomac Organization, Inc.
5400 Greystone St.
Chevy Chase, MD 20815

Maris Vinovskis
Institute for Social Research
Room 4086
University of Michigan
426 Thompson St
Ann Arbor, MI 48109-1045

Gregory Benford
University of California, Irvine
Department of Physics
Irvine, CA 92717

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Tempe, AZ 85287

Harry Otway
Health, Safety, and Envir. Div.
Mail Stop K-491
Los Alamos National Laboratory
Los Alamos, NM 87545

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Department of Geography
Arizona State University
Tempe, AZ 85287-3806

Michael Baram
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33 Mount Vernon St.
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FEDERAL REPUBLIC OF GERMANY

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Forschungsgelände
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FEDERAL REPUBLIC OF GERMANY

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JAPAN

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Cátedra de Tecnología Nuclear
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José Gutiérrez Abascal, 2
E-28006 Madrid
SPAIN

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CIEMAT
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Avenida Complutense, 22
E-28040 Madrid
SPAIN

Miguel Angel Cuñado
ENRESA
Emilio Vargas, 7
E-28043 Madrid
SPAIN

Francisco Javier Elorza
ENRESA
Emilio Vargas, 7
E-28043 Madrid
SPAIN

Nils A. Kjellbert
Swedish Nuclear Fuel and Waste Management Company (SKB)
Box 5864
S-102 48 Stockholm
SWEDEN

Björn Cronhjort
Swedish National Board for Spent Nuclear Fuel (SKN)
Sehlsedtsgatan 9
S-115 28 Stockholm
SWEDEN

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SWITZERLAND

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Department of the Environment
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Room A5.33, Romney House
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45 Station Road
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UNITED KINGDOM

Richard Codell
U.S. Nuclear Regulatory Commission
Mail Stop 4-H-3
Washington, D.C. 20555

Norm A. Eisenberg
Division of High Level Waste Management
Office of Nuclear Material Safety and Safeguards
Mail Stop 4-H-3
Washington, D.C. 20555

Paul W. Eslinger
Battelle Pacific Northwest Laboratories (PNL)
P.O. Box 999, MS K2-32
Richland, WA 99352

Budhi Sagar
Center for Nuclear Waste Regulatory Analyses (CNWRA)
Southwest Research Institute
Post Office Drawer 28510
6220 Culebra Road
San Antonio, TX 78284

Andrea Saltelli
Commission of the European Communities
Joint Research Centre od Ispra
I-21020 Ispra (Varese)
ITALY

Shaheed Hossain
Division of Nuclear Fuel Cycle and Waste Management
International Atomic Energy Agency
Wagramerstrasse 5
P.O. Box 100
A-1400 Vienna
AUSTRIA

Daniel A. Galson
Division of Radiation Protection and Waste Management
38, Boulevard Suchet
F-75016 Paris
FRANCE

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ROE 1L0

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800 Kipling Avenue
Toronto, Ontario, CANADA
M8Z 5S4

Ghislain de Marsily
Lab. Géologie Appliqué
Tour 26, 5 étage
4 Place Jussieu
F-75252 Paris Cedex 05, FRANCE

Jean-Pierre Olivier
OECD Nuclear Energy Agency (2)
38, Boulevard Suchet
F-75016 Paris, FRANCE

D. Alexandre, Deputy Director
ANDRA
31 Rue de la Federation
75015 Paris, FRANCE

Claude Sombret
Centre D'Etudes Nucleaires
De La Vallee Rhone
CEN/VALRHO
S.D.H.A. BP 171
30205 Bagnols-Sur-Ceze
FRANCE

Bundesministerium fur Forschung und
Technologie
Postfach 200 706
5300 Bonn 2
FEDERAL REPUBLIC OF GERMANY

Bundesanstalt fur Geowissenschaften
und Rohstoffe
Attn: Michael Langer
Postfach 510 153
3000 Hannover 51
FEDERAL REPUBLIC OF GERMANY

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FEDERAL REPUBLIC OF GERMANY

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Theodor-Heuss-Strasse 4
D-3300 Braunschweig
FEDERAL REPUPLIC OF GERMANY

Kernforschung Karlsruhe
Attn: K. D. Closs
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7500 Karlsruhe
FEDERAL REPUBLIC OF GERMANY

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Postfach 33 45
D-3300 Braunschweig
FEDERAL REPUBLIC OF GERMANY

D. R. Knowles
British Nuclear Fuels, plc
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Shingo Tashiro
Japan Atomic Energy Research
Institute
Tokai-Mura, Ibaraki-Ken
319-11 JAPAN

Netherlands Energy Research
Foundation
ECN (2)
Attn: Tuen Deboer, Mgr.
L. H. Vons
3 Westerduinweg
P.O. Box 1
1755 ZG Petten, THE NETHERLANDS

Johan Andersson
Statens Kärnkraftinspektion
SKI
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GLOSSARY

ccdf - see complementary cumulative distribution function.

cdf - see cumulative distribution function.

complementary cumulative distribution function (CCDF) - One minus the cumulative distribution function.

Culebra Dolomite Member - The lower of two layers of dolomite within the Rustler Formation that are locally water bearing.

cumulative distribution function - The sum (or integral as appropriate) of the probability of those values of a random variable that are less than or equal to a specified value.

empirical - Relying explicitly upon or derived explicitly from observation or experiment.

exponential distribution - A probability distribution whose PDF is an exponential function defined on the range of the variable in question.

hydraulic conductivity - The measure of the rate of flow of water through a unit cross-sectional area under a unit hydraulic gradient.

lognormal distribution - A probability distribution in which the logarithm of the variable in question follows a normal distribution.

loguniform distribution - A probability distribution in which the logarithm of the variable in question follows a uniform distribution.

mean - The expectation of a random variable; i.e., the sum (or integral) of the product of the variable and the PDF over the range of the variable.

median - That value of a random variable at which its CDF takes the value 0.5; i.e., the 50^{th} percentile point.

mode - That value of a random variable at which its PDF takes its maximum value.

normal distribution - A probability distribution in which the PDF is a symmetric, bell-shaped curve of bounded amplitude extending from minus infinity to plus infinity.

PDF - see probability density function.

porosity - The percentage of total rock volume occupied by voids.

probability density function - For a continuous random variable X, the function giving the probability that X lies in the interval x to x + dx centered about a specified value x.

solubility - The equilibrium concentration of a solute when undissolved solute is in contact with the solution.

subjective - The opposite of empirical: not supported by explicit records of measurements or experiments.

tortuosity - A measure of the actual length of the path of flow through a porous medium.

truncated distribution - A probability distribution whose curve is defined on a range of variable values that is smaller than the range normally associated with the distribution: e.g., a normal distribution defined on a finite range of variable values.

uniform distribution - A probability distribution in which the PDF is constant over the range of variable values.

variance - The square of the standard deviation of a probability distribution; the standard deviation is a measure of the amount of spreading of a PDF about its mean.

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