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Mathematical and Numerical Approaches in Performance Assessment for Radioactive Waste Disposal: Dealing with Uncertainty

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1. Introduction

In the context of this presentation, performance assessment (PA) is used to indicate an analysis intended to answer the following questions about a natural or engineered system: Q1, "What occurrences can take place?"; Q2, "How likely are these occurrences?"; Q3, "What are the consequences of individual occurrences?"; and Q4, "How much confidence exists in the answers to the first three questions (i.e., Q1 - Q3)?"

Performance assessment for radioactive waste disposal is a topic of wide national and international interest.[1-4] As examples, major radioactive waste disposal programs exist in the United States (i.e., the Waste Isolation Pilot Plant (WIPP)[5, 6] and the Yucca Mountain Project[7]), Canada,[8] Sweden,[9] and France.[10] This presentation will be illustrated primarily with results from PAs carried out for the WIPP. However, the ideas under consideration are quite general and apply not only to PAs for radioactive waste disposal facilities but also to PAs for other complex systems such as nuclear power plants, chemical production facilities, and transportation systems.

A central focus of this presentation is how uncertainty should be treated in a PA for a radioactive waste disposal facility or some other complex system. In such assessments, uncertainty is often divided into two components: (i) stochastic or aleatory uncertainty, which arises because the system under study can potentially behave in many different ways, and (ii) subjective or epistemic uncertainty, which arises from a lack of knowledge about quantities that are assumed to have fixed values within the computational implementation of the PA.[11-16] The use of probability to quantify these two classifications of uncertainty can be traced to the beginnings of the formal development of probability in the seventeenth century.[17, 18] In the context of the previously indicated questions, stochastic uncertainty relates to Q1 and Q2, and subjective uncertainty relates to Q4.

A PA can be discussed at an intuitive and informal level. For example, describing a PA as an attempt to answer questions Q1 - Q4 is an example of such usage. For many descriptive purposes, such informality is appropriate. However, the actual computational implementation of a PA requires a careful mathematical description of what is to

be done; without such a description, it is difficult to produce a coherent analysis. Indeed, given that PAs invariably involve mathematical calculations, an inability to produce a formal description of the mathematical approaches in use suggests an analysis that has not been carefully thought through. Further, meaningful review of a PA also requires a careful mathematical description of the analysis; without such a description, it is difficult to communicate to reviewers what was done in the analysis. Descriptions of the mathematical approaches in use are required on at least three levels: (i) overall structure of analysis, (ii) probabilistic characterization of uncertainty, and (iii) representation of individual physical processes.

Three distinct entities typically underlie the mathematical approaches used in a performance assessment: EN1, a probabilistic characterization of what could occur at the site under consideration; EN2, mathematical models for estimating the consequences of what could occur; and EN3, a probabilistic characterization of the uncertainty in the parameters used in the definitions of EN1 and EN2. The term parameter in the definition of EN3 is used broadly enough to include designators for alternative models or model structures. At a formal level, EN1 and EN3 are suitably defined probability spaces, and EN3 often consists of systems of ordinary or partial differential equations used to represent various physical processes. In the context of the previously indicated questions, EN1 is providing the answer to Q1 and Q2; EN2 is providing the answer to Q3; and EN3 is providing the answer to Q4.

Careful definition of EN1, EN2 and EN3 leads to a description of the mathematical approaches being used in a PA. However, this description is typically at a formal level (i.e., as integrals involving probability spaces and solutions to ordinary or partial differential equations). The actual production of numerical results also requires both procedures for approximating the mathematical structures used in the description of the PA and computer software for the implementation of these procedures. The quality of these procedures and the implementing software can have a significant effect on the practicability of the analysis and the correctness of the final results.

2. Screening of Features, Events and Processes (FEPs)

A PA should be based on a well-defined structure in which both the mathematical components of the analysis and their numerical approximations can be unambiguously specified. However, a PA does not start out well-defined. Rather, some type of procedure must be used to decide what is to be incorporated into, and excluded from, the analysis. This process is often referred to as the screening of features, events and processes (FEPs). Once the screening of FEPs is completed, the more formal structure of the analysis as embodied in EN1, EN2 and EN3 can be developed.

In practice, most important FEPs will probably be identified without the use of any formal process by the time that the development of a radioactive waste disposal facility has reached the point that a formal PA is required. However, to satisfy public concerns and regulatory requirements, a formal procedure may be called for that provides

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a systematic development and description of the selection process used to determine what is to be included in the PA. For example, the following requirement appears in the regulations that apply to the WIPP (Ref. 19, p. 5242):

> § 194.32 Scope of performance assessments.
> . . . (e) Any compliance application(s) shall include information which: (1) identifies all potential processes, events or sequences and combinations of processes and events that may occur during the regulatory time frame and may affect the disposal system; (2) Identifies the processes, events or sequences and combinations of processes and events included in performance assessments; and (3) Documents why any processes, events or sequences and combinations of processes and events identified pursuant to paragraph (e)(1) of this section were not included in performance assessment results provided in any compliance application.

The 1996 WIPP PA provides an example of a real analysis in which an extensive screening of FEPs was carried out. As a starting point, a list of potentially relevant FEPs was assembled from a compilation developed for the Swedish Nuclear Power Inspectorate (SKI).[20] The SKI list is based on several FEP lists developed for other waste disposal programs[21-27] and constituted the best documented and most comprehensive starting point for the WIPP PA. WIPP-specific FEPs were added to the SKI list, and the combined list was edited to remove redundancy and ambiguity, resulting in a FEPs list (Ref. 28, Attachment 1, Appendix SCR) that was appropriate for the WIPP (Ref. 28, Section 6.2.1).

This list was then carefully analyzed to identify the FEPs that should be incorporated into the computational structure of the 1996 WIPP PA and also the FEPs that did not require incorporation into this structure. Decisions to remove (i.e., screen out) FEPs from the computational structure used for the 1996 WIPP PA were based on the following criteria: regulatory exclusion (SO-R), low probability (SO-P), and low consequence (SO-C). The three screening criteria derive from specific regulatory requirements (Ref. 28, Section 6.2.1).

The FEPs not screened out were retained for inclusion in the PA and were classified as undisturbed performance (UP) or disturbed performance (DP) FEPs. As an example, a summary of the screening process for natural FEPs is given in Table 1; in addition, waste- and repository-induced FEPs (Ref. 28, Table 6-46) and human-initiated events and processes (EPs) (Ref. 28, Table 6-56) were also considered. A detailed description of the screening process is available in Appendix SCR of Ref. 28.

3. EN1: Probabilistic Characterization of Different Futures

An important outcome of the FEPs process is an identification of occurrences (e.g., volcanism, faulting, human disruption, ...) that could take place with sufficient likelihood and consequence to merit inclusion in a PA for the facility under consideration. Typically, these occurrences are constrained to take place over some time interval of interest (e.g., 10,000 yr in the regulations that apply to the WIPP). There are two aspects to the specification of such

occurrences: (i) definition of occurrence properties (e.g., time, location, magnitude, ...) within the time interval of interest, and (ii) assignment of probabilities to possible occurrences within the time interval of interest.

The assignment of probabilities is only necessary if some form of probabilistic presentation of results is to be used. If results are presented conditional on individual occurrences, then probabilities are not needed. However, presumably even in this case, some sort of probabilistic selection is taking place as there would be little purpose in analyzing a group of occurrences that had a probability of zero of taking place. For the following discussion, the assumption is made that probabilities are to be assigned to future occurrences.

The development of probabilities requires a careful specification of exactly what probabilities are to be assigned to. As an example, suppose only two occurrences, designated o_1 and o_2, with the following properties were selected for inclusion in a PA: (i) the occurrences of o_1 and o_2 are independent, (ii) the occurrences of o_1 and o_2 follow Poisson processes with rate constants λ_1 (yr^{-1}) and λ_2 (yr^{-1}), respectively, and (iii) a time interval [0, T = 1000 yr] is under consideration. There are many possible patterns of occurrence of o_1 and o_2 over the interval [0, T]. Each possible pattern can be represented by a vector

$$\mathbf{x} = [t_{11}, t_{12}, \ldots, t_{1m}, t_{21}, t_{22}, \ldots, t_{2n}] \tag{1}$$

where

$$0 \le t_{11} \le t_{12} \le \ldots \le t_{1m} \le T = 1000 \text{ yr}$$

$$0 \le t_{21} \le t_{22} \le \ldots \le t_{2n} \le T = 1000 \text{ yr}$$

and t_{1i}, $i = 1, 2, \ldots, m$, and t_{2j}, $j = 1, 2, \ldots, n$, are times at which o_1 and o_2, respectively, take place.

Each vector $\mathbf{x}$ in Eq. (1) represents a possible pattern of occurrences over the time interval [0, T]. The pattern of occurrences characterized by $\mathbf{x}$ is sometimes referred to as a future in radioactive waste disposal because each $\mathbf{x}$ is describing one possible future at the facility under consideration. The set

$$\mathcal{S} = \{\mathbf{x} : \mathbf{x} \text{ a vector in Eq. (1)}\} \tag{2}$$

corresponds to the universe of all possible futures that could occur over the time interval [0, T] given the assumption that o_1 and o_2 are the only two occurrences to be considered.

The introduction of $\mathbf{x}$ provides an exact mathematical description (i.e., definition) of occurrence properties within the time interval of interest. The vector $\mathbf{x}$ in Eq. (1) is quite simple; in general, more properties than initiation times are required to define individual occurrences in a PA. A more general formulation of the example would be

$$\mathbf{x} = [\mathbf{o}_{11}, \mathbf{o}_{12}, \ldots, \mathbf{o}_{1m}, \mathbf{o}_{21}, \mathbf{o}_{22}, \ldots, \mathbf{o}_{2n}] \tag{3}$$

where $\mathbf{o}_{1i}$, $i = 1, 2, \ldots, m$, and $\mathbf{o}_{2j}$, $j = 1, 2, \ldots, n$, are vectors of properties associated with the occurrence of o_1 and o_2. Further, PAs can involve more than two occurrences of interest. However, $\mathbf{x}$ as defined in Eq. (1) is sufficient as an example.

The assignment of probabilities is now considered. Typically, individual futures of the form illustrated by $\mathbf{x}$ in Eq. (1) have a probability of zero. Thus, probabilities are usually used in reference to sets of futures or, equivalently, to subsets $\mathcal{E}$ of $\mathcal{S}$ in Eq. (2). For example, $\mathcal{E}$ might be defined by

$$\mathcal{E} = \{\mathbf{x} = [t_{11}, t_{21}, t_{22}] : 0 \le t_{11} \le 500 \text{ yr}, 0 \le t_{21} \le t_{22} \le 1000 \text{ yr}\}. \tag{4}$$

Then, under the previously stated assumptions that o_1 and o_2 are independent and follow Poisson processes with rate constants λ_1 and λ_2, the probability $p(\mathcal{E})$ of $\mathcal{E}$ is given by

$$p(\mathcal{E}) = \{[(500\lambda_1)^1/1!][\exp(-500\lambda_1)]\}\{\exp(-500\lambda_1)\}\{[(1000\lambda_2)^2/2!][\exp(-1000\lambda_2)]\}. \tag{5}$$

Thus, in this example and more generally in most situations, probability distributions are introduced for the individual elements of $\mathbf{x}$ and then used to define probabilities for sets of $\mathbf{x}$. The closed form calculation of such probabilities can be difficult or impossible; often, Monte Carlo techniques or other numerical procedures must be used to calculate approximate probabilities.

To the extent practicable, descriptions of the various parts of a PA should use widely recognized mathematical constructions. Then, the computational implementation of the PA can be viewed as the calculation of approximations to these constructions. For probability, the fundamental mathematical construction is a probability space, which involves three components: (i) a set $\mathcal{S}$ that contains everything that could occur in the particular universe under consideration, (ii) a set $\mathcal{A}$ of subsets of $\mathcal{S}$, and (iii) a function p that defines the probability of the individual elements of $\mathcal{A}$ (p. 116, Ref. 30). The preceding three components appear in the previous example. In the terminology of probability theory, $\mathcal{S}$ is the sample space; elements $\mathbf{x}$ of $\mathcal{S}$ are elementary events; elements $\mathcal{E}$ of $\mathcal{A}$ are events; p is a probability measure; and the triple $(\mathcal{S}, \mathcal{A}, p)$ is a probability space. In terminology often used in PA for radioactive waste disposal, elements $\mathbf{x}$ of $\mathcal{S}$ are futures; elements $\mathcal{E}$ of $\mathcal{A}$ are scenarios; the probabilities $p(\mathcal{E})$ are scenario probabilities; and questions of "completeness" deal with whether or not $\mathcal{S}$ has been defined in a way that incorporates all significant occurrences at the site under consideration.

In practice, most probability calculations are based on the distributions assigned to the individual elements of $\mathbf{x}$ and do not rely on the formal properties of the probability space $(\mathcal{S}, \mathcal{A}, p)$. However, the introduction of the concept of a probability space provides a way to formally describe what is being done in a PA and also a way to distinguish between different uses of probability within a PA.

As indicated in Sect. 1, uncertainty about occurrences that may take place in the future is often designated stochastic or aleatory uncertainty. Thus, the probabilistic characterization of different possible futures in a PA involves stochastic uncertainty. For this reason, the subscript *st* is sometimes added to vectors $\mathbf{x}$ of the form illustrated in Eq. (1) (i.e., $\mathbf{x}_{st}$ replaces $\mathbf{x}$) to indicate that these vectors are being used in the characterization of stochastic uncertainty. Correspondingly, $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ is used instead of $(\mathcal{S}, \mathcal{A}, p)$ to indicate the characterization of stochastic uncertainty. The probability space $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ is providing a probabilistic characterization of the different futures that could occur at the facility under consideration and formally defines the entity EN1 referred to in Sect. 1 and the heading to this section.

Results from the 1996 WIPP PA are now used for illustration. The FEPs development process for the WIPP identified exploratory drilling for natural resources as the only disruption with sufficient likelihood and consequence for inclusion in the definition of EN1 (App. SCR, Ref. 28). In addition, regulatory requirements[19] specify that the occurrence of potash mining near the site must be included in the analysis. The preceding considerations led to the elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$ being vectors of the form

$$\mathbf{x}_{st} = [\underbrace{t_1, l_1, e_1, b_1, p_1, \mathbf{a}_1}_{1^{\text{st}}\text{ intrusion}}, \underbrace{t_2, l_2, e_2, b_2, p_2, \mathbf{a}_2}_{2^{\text{nd}}\text{ intrusion}}, \ldots, \underbrace{t_n, l_n, e_n, b_n, p_n, \mathbf{a}_n}_{n^{\text{th}}\text{ intrusion}}, t_{min}] \tag{6}$$

in the 1996 WIPP PA, where n is the number of drilling intrusions in the vicinity of the WIPP, t_i is the time (yr) of the i^{th} intrusion, l_i designates the location of the i^{th} intrusion, e_i designates the penetration of an excavated or nonexcavated area by the i^{th} intrusion, b_i designates whether or not the i^{th} intrusion penetrates pressurized brine in the Castile Formation, p_i designates the plugging procedure used with the i^{th} intrusion (i.e., continuous plug, two discrete plugs, three discrete plugs), $\mathbf{a}_i$ designates the type of waste penetrated by the i^{th} intrusion (i.e., no waste, contact-handled (CH) waste, remotely-handled (RH) waste), and t_{min} is the time at which potash mining occurs.

In the development of $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$, the probabilistic characterization of n, t_i, l_i, and e_i derives from the assumption that drilling intrusions occur randomly in time and space (i.e., follow a Poisson process); the probabilistic characterization of b_i derives from assessed properties of brine pockets; the probabilistic characterization of $\mathbf{a}_i$ derives from the properties of the waste to be emplaced at the WIPP; and the probabilistic characterization of p_i derives from current drilling practices in the sedimentary basin in which the WIPP is located. A vector notation is used for $\mathbf{a}_i$ because a given drilling intrusion can penetrate several different types of waste. Further, the probabilistic characterization for t_{min} follows from regulatory guidance that the occurrence of potash mining should be assumed to occur randomly in time (i.e., follow a Poisson process with a rate constant of $\lambda_m = 10^{-4}$ yr^{-1}), with all commercially viable potash reserves being extracted at time t_{min}. Additional information on $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ is given in Chapt. 3 of Ref. 31.

4. EN2: Mathematical Models for Estimating Consequences of Individual Futures

The entity EN2 corresponds to the mathematical models required to estimate various consequences in a PA for a radioactive waste disposal site or some other facility. Conceptually, EN2 can be viewed as a function **f** of the form

$$\mathbf{y} = \mathbf{f}(\mathbf{x}_{st}), \tag{7}$$

where $\mathbf{x}_{st}$ is a particular future, **f** corresponds to the models used to estimate various outcomes associated with $\mathbf{x}_{st}$, and **y** is the estimated outcomes. A vector notation is used for **f** and **y** because typically a large number of outcomes is estimated for each future $\mathbf{x}_{st}$. For a radioactive waste disposal site, the models denoted by **f** are often systems of ordinary or partial differential equations used to represent processes such as material deformation, corrosion, fluid flow, radionuclide transport in flowing groundwater, and radionuclide movement and associated human radiation exposure in the surface environment.

The models used in a particular PA will depend on many things, including the site under consideration, the resolution of the data available for characterization of the site, the desired resolution in model predictions, and the time and resources available for the analysis. However, most models will consist of three parts: (i) a formal mathematical representation (e.g., a system of nonlinear partial differential equations), (ii) a numerical procedure that produces approximations to the formal mathematical representation (e.g., a finite difference procedure; see Chapt. 19, Ref. 32), and (iii) a computer program that implements the numerical procedure.

Given the almost universal use of numerical approximations and computer programs to implement these approximations, a PA typically involves two extensions of the representation in Eq. (7):

$$\mathbf{y} = \hat{\mathbf{f}}(\mathbf{x}_{st}) \tag{8}$$

$$\mathbf{y} = \mathbf{F}(\mathbf{x}_{st}), \tag{9}$$

where $\hat{\mathbf{f}}$ is used to represent the numerical approximation that replaces **f**, and **F** is used to represent the computer program that implements this approximation and actually produces **y**. For example, if **f** was based on a system of ordinary differential equations, $\hat{\mathbf{f}}$ might correspond to an Adams-Moulten method, a variable order, variable stepsize Runge-Kutta method or a Gear's backward differentiation method, and **F** would correspond to the program that actually implemented the method (Chapt. 16, Ref. 32). The absence of good numerical procedures and their appropriate implementation can lead to (i) excessive computational times, (ii) erroneous results, and (iii) possibly no results at all.

Models used in the 1996 WIPP PA to estimate total normalized radionuclide release to the accessible environment are now used for illustration, where normalized release refers to a single release value derived from the

releases of several radionuclides on the basis of the initial radionuclide inventory in the repository and the radiological hazard of the individual radionuclides (Sect. 2, Ref. 5). In this example, f is real valued and has the form

$$f(\mathbf{x}_{st}) = f_C(\mathbf{x}_{st}) + f_{SP}\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right] + f_{DBR}\left\{\mathbf{x}_{st}, f_{SP}\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right], \mathbf{f}_B(\mathbf{x}_{st})\right\}$$

$$+ f_{MB}\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right] + f_{DL}\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right] + f_S\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right]$$

$$+ f_{S-T}\left\{\mathbf{x}_{st,0}, \mathbf{f}_{S-F}\left(\mathbf{x}_{st,0}\right), \mathbf{f}_{N-P}\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right]\right\}, \tag{10}$$

where $\mathbf{x}_{st}$ ~ particular future under consideration, $\mathbf{x}_{st,0}$ ~ future involving no drilling intrusions but a mining event at the same time t_{min} as in $\mathbf{x}_{st}$, $f_C(\mathbf{x}_{st})$ ~ cuttings and cavings release to accessible environment calculated with the CUTTINGS_S program, $\mathbf{f}_B(\mathbf{x}_{st})$ ~ two-phase flow results calculated with the BRAGFLO program, $\mathbf{f}_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ spallings release to accessible environment calculated with the CUTTINGS_S program, $f_{DBR}\{\mathbf{x}_{st}, f_{SP}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})], \mathbf{f}_B(\mathbf{x}_{st})\}$ ~ direct brine release to accessible environment calculated with the BRAGFLO_DBR program, $f_{MB}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})]$ ~ release through anhydrite marker beds to accessible environment calculated with the NUTS program, $f_{DL}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})]$ ~ release through Dewey Lake Red Beds to accessible environment calculated with the NUTS program, $f_S[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})]$ ~ release to land surface due to brine flow up a plugged borehole with the NUTS or PANEL program as appropriate, $\mathbf{f}_{S-F}\left(\mathbf{x}_{st,0}\right)$ ~ Culebra flow field calculated with the SECOFL2D program, $\mathbf{f}_{N-P}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})]$ ~ releases to Culebra calculated with the NUTS or PANEL program as appropriate, $f_{S-T}\{\mathbf{x}_{st,0}, \mathbf{f}_{S-F}(\mathbf{x}_{st,0}), \mathbf{f}_{N-P}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})]\}$ ~ groundwater transport release through Culebra to accessible environment calculated with the SECOTP2D program. Although f is shown as being real valued in Eq. (10) because a single analysis outcome is under consideration, the 1996 WIPP PA was quite complex and a description of the analysis in full generality would require use of vector representations for all models.

As indicated in Table 2, each model actually consists of a formal mathematical structure (typically a system of ordinary or partial differential equations), a numerical procedure for approximating this structure, and an implementing computer program. The 1996 WIPP PA is typical of large PAs in that f does not correspond to a single model, but rather an ensemble of models that is used to produce results of interest.

5. Combining EN1 and EN2: Complementary Cumulative Distribution Functions (CCDFs)

In a PA, EN1 (i.e., the probability space $(S_{st}, \mathcal{A}_{st}, p_{st})$) provides a probabilistic characterization of what could happen at the facility under consideration, and EN2 (i.e., the function $\mathbf{f}$ indicated in Eq. (7)) provides an estimate of the consequences associated with individual futures $\mathbf{x}_{st}$. In many PAs, a representation of results is desired that

provides a display of both consequence and likelihood. The usual mathematical construction used to display this information is a CCDF, which provides a display of the probability that individual consequence values will be exceeded (Fig. 1).

A CCDF can be formally defined by an integral involving EN1 and EN2. Specifically,

$$prob(c > C) = \int_{S_{st}} \delta_C[f(\mathbf{x}_{st})] d_{st}(\mathbf{x}_{st}) dV_{st}, \tag{11}$$

where $prob(c > C)$ is the probability that a future $\mathbf{x}_{st}$ yielding a consequence value larger than C will occur, $d_{st}(\mathbf{x}_{st})$ is the density function associated with $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$, dV_{st} is an incremental (i.e., differential) volume from $\mathcal{S}_{st}$,

$$\delta_C[f(\mathbf{x}_{st})] = \begin{cases} 1 \text{ if } f(\mathbf{x}_{st}) > C \\ 0 \text{ if } f(\mathbf{x}_{st}) \le C \end{cases}$$

and a nonbold representation for f is used because a single consequence (i.e., analysis outcome) is considered in the construction of a CCDF (i.e., f is real valued rather than vector valued in this context). The effect of the indicator function δ_C is to pick out the subset of $\mathcal{S}_{st}$ for which $f(\mathbf{x}_{st}) > C$, with the result that the integral yields the desired probability. To be fully general, the preceding integral should be shown as a Lebesgue integral (App. B, Ref. 34); however, notation associated with the more familiar Riemann integral has been used for simplicity.

In practice, the integral in Eq. (11) is too complex to permit a closed-form evaluation. Part of this complexity comes from the properties of $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ (e.g., see Eq. (6)) and part of it comes from the complexity of f (e.g., see Eq. (10)). This complexity typically precludes the use of standard numerical procedures for evaluating integrals. In practice, either Monte Carlo techniques or importance sampling is used in the evaluation of the integral in Eq. (11).

With the Monte Carlo approach, the integral in Eq. (11) is approximated by

$$prob(c > C) \doteq \sum_{i=1}^{nR} \delta_C[f(\mathbf{x}_{st,i})] / nR, \tag{12}$$

where $\mathbf{x}_{st,i}$, $i = 1, 2, \ldots, nR$, is a random sample from $\mathcal{S}_{st}$ generated in consistency with the definition of $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ (Fig. 2). In practice, generating a random sample from $\mathcal{S}_{st}$ in consistency with the definition of $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ means generating a sample using the distributions assigned to the individual elements of $\mathbf{x}_{st}$ (e.g., see $\mathbf{x}_{st}$ in Eq. (6) and associated discussion).

In most PAs, evaluation of $f(\mathbf{x}_{st})$ is too expensive to permit an evaluation for each sample element $\mathbf{x}_{st,i}$ in Eq. (12). Rather, $f(\mathbf{x}_{st})$ is evaluated for a relatively small number of elements of $\mathcal{S}_{st}$ and then these evaluations are used in the construction (i.e., approximation) of $f(\mathbf{x}_{st,i})$ for use in the summation in Eq. (12). Thus, there are actually three numerical approximations involved: (i) the Monte Carlo procedure to approximate the integral in Eq. (11), (ii) an

initial approximation of $f(\mathbf{x}_{st})$ for selected elements of $\mathcal{S}_{st}$, and (iii) a subsequent approximation of $f(\mathbf{x}_{st,i})$ from these initial approximations for use in the summation in Eq. (12). As an example, the procedures used in the 1996 WIPP PA to estimate the CCDF for

$$f(\mathbf{x}_{st}) = f_{SP}\left[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})\right] \tag{13}$$

(i.e., the CCDF for the spallings release calculated by the program CUTTINGS_S) are described in Sect. 9 of Ref. 5.

With importance sampling, $\mathcal{S}_{st}$ is divided into strata $\mathcal{S}_{st,i}$, $i = 1, 2, \ldots, nS$, and a value $\mathbf{x}_{st,i}$, $i = 1, 2, \ldots, nS$, is selected from each strata. Then, the integral in Eq. (11) is approximated by

$$prob(c > C) \doteq \sum_{i=1}^{nS} \delta_C[f(\mathbf{x}_{st,i})]\, p_{st}(\mathcal{S}_{st,i}), \tag{14}$$

where $p_{st}(\mathcal{S}_{st,i})$ is the probability of $\mathcal{S}_{st,i}$. When the $\mathbf{x}_{st,i}$ are randomly selected within the corresponding strata, importance sampling is a variance reduction technique for simple random (i.e., Monte Carlo) sampling. Importance sampling involves the same approximation considerations as the Monte Carlo approach described in conjunction with Eq. (12). The fault tree and event tree techniques[35, 36] used extensively in conjunction with PAs for nuclear reactors and other complex engineered systems can be viewed as algorithms for defining an importance sampling procedure over the sample space associated with all possible accidents at these facilities. Several early PAs for the WIPP used an importance sampling procedure in CCDF construction.[37]

Another possible display of the combined effects of EN1 and EN2 is given by the expected value and variance of a consequence of interest. The expected value $E(f)$ and variance $V(f)$ of a particular consequence are formally defined by

$$E(f) = \int_{\mathcal{S}_{st}} f(\mathbf{x}_{st}) d_{st}(\mathbf{x}_{st}) dV_{st} \tag{15}$$

and

$$V(f) = \int_{\mathcal{S}_{st}} [f(\mathbf{x}_{st}) - E(f)]^2 d_{st}(\mathbf{x}_{st}) dV_{st} \tag{16}$$

and are easily estimated with the results used in the CCDF approximations in Eqs. (12) and (14). However, as a large amount of information is lost in the calculation of $E(f)$ and $V(f)$, the combined effects of EN1 and EN2 are better displayed as CCDFs.

6.0 EN3: Probabilistic Characterization of Parameter Uncertainty

The entity EN3 is the formal outcome of the data development component of a PA and provides a probabilistic characterization of the uncertainty in the many parameters required in the definitions of EN1 (e.g., occurrence rates, parameters in distributions, ...) and EN2 (e.g., distribution coefficients, solubilities, ...). The term parameter in the description of EN3 is used in a sense that is sufficiently broad to include designators for alternative models or model structures. Formally, EN3 is defined by a probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$, with the subscript *su* selected to indicate subjective (i.e., epistemic) uncertainty.

The sample space $\mathcal{S}_{su}$ associated with EN3 has the form

$$\mathcal{S}_{su} = \{\mathbf{x}_{su} : \mathbf{x}_{su} \text{ is possibly the correct vector of inputs to use with EN1 and EN2 in the calculation of analysis outcomes}\}. \quad (17)$$

Further, $\mathbf{x}_{su}$ has the form

$$\mathbf{x}_{su} = [x_1, x_2, \ldots, x_{nV}], \quad (18)$$

where each element x_i, $i = 1, 2, \ldots, nV$, of $\mathbf{x}_{su}$ is quantity required in the formulation of EN1 or EN2 that is assumed to have a fixed value in the context of the particular PA under consideration but with this value being imprecisely known. The basic idea is that the PA and the associated definitions of EN1 and EN2 have been developed to the point that appropriate analysis outcomes would be obtained if the appropriate value of $\mathbf{x}_{su}$ was used as input to the analysis.

As an example, the representation for the CCDF in Eq. (11) would now become

$$prob(c > C \mid \mathbf{x}_{su}) = \int_{\mathcal{S}_{st}(\mathbf{x}_{su})} \delta_C[f(\mathbf{x}_{st}, \mathbf{x}_{su})] d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su}) dV_{st}, \quad (19)$$

with the addition of $\mathbf{x}_{su}$ to the notation for various quantities in Eq. (11) indicating that the values and/or predictions associated with these quantities are dependent on the value assigned to $\mathbf{x}_{su}$. Thus, different values for $\mathbf{x}_{su}$ lead to different values for the CCDF in Eq. (11) and other analysis outcomes of interest (Fig. 3). The sample space $\mathcal{S}_{su}$ contains all values for $\mathbf{x}_{su}$ consistent with available information about the facility under consideration and thus leads to all possible values for the CCDF defined in Eq. (11) and other analysis outcomes of interest.

The probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ that formally defines EN3 provides a characterization of the uncertainty in the elements of $\mathbf{x}_{su}$. In practice, $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ is defined by specifying a distribution

$$D_j, j = 1, 2, \ldots, nV, \quad (20)$$

for each element x_j of $\mathbf{x}_{su}$. Correlations and various other restrictions involving the possible values of x_j can also be specified. The purpose of the D_j is to provide, on the basis of all available information, a quantitative (i.e., probabilistic) description of where the possible values for the x_j are located. In contrast, S_{su} only provides a complete compilation of the possible values for the $\mathbf{x}_{su}$ and thus for the x_j. In some instances, it may be possible to use formal statistical procedures to estimate the D_j. However, typically some type of expert review process is needed to develop the D_j.[24, 38-43]

As an example, the 1996 WIPP PA considered $nV = 57$ uncertain variables, with the result that $\mathbf{x}_{su}$ had the form

$$\begin{aligned}\mathbf{x}_{su} &= [x_1, x_2, \ldots, x_{57}] \\ &= [ANHPRM, BHPRM, \ldots, WTAUFAIL].\end{aligned} \tag{21}$$

Example elements of $\mathbf{x}_{su}$ are given in Table 3. In concept, elements of $\mathbf{x}_{su}$ can affect the definition of EN1 (i.e., the probability space $(S_{st}, \mathcal{A}_{st}, p_{st})$) or the definition of EN2 (i.e., the function $\mathbf{f}$ in Eq. (7)). In the 1996 WIPP PA, the elements of $\mathbf{x}_{su}$ only affected EN2. However, in a subsequent PA carried out at the request of the U.S. Environmental Protection Agency, the probability of penetrating pressurized brine in the Castile Formation was treated as being uncertain (see b_i in Eq. (6)) and so the analysis incorporated subjective uncertainty in the definition of $(S_{st}, \mathcal{A}_{st}, p_{st})$.[44]

For a specific future $\mathbf{x}_{st}$ and a single analysis outcome $f(\mathbf{x}_{st}, \mathbf{x}_{su})$, the resultant distribution of possible values for $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ is given by

$$prob(c > C \mid \mathbf{x}_{st}) = \int_{S_{su}} \delta_C[f(\mathbf{x}_{st}, \mathbf{x}_{su})] d_{su}(\mathbf{x}_{su}) dV_{su}, \tag{22}$$

where $prob(c > C|\mathbf{x}_{st})$ is the probability that $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ will have a value larger than C due to the uncertainty in $\mathbf{x}_{su}$ as characterized by $(S_{su}, \mathcal{A}_{su}, p_{su})$ and the remaining terms are defined similarly to those in Eqs. (11) and (19) except that $(S_{su}, \mathcal{A}_{su}, p_{su})$ rather than $(S_{st}, \mathcal{A}_{st}, p_{st})$ is now under consideration. In concept, this distribution has the same appearance as in Fig. 1 except that $C = f(\mathbf{x}_{st}, \mathbf{x}_{su})$ appears on the abscissa and $prob(c > C|\mathbf{x}_{st})$ appears on the ordinate.

In practice, closed form evaluation of $prob(c > C|\mathbf{x}_{st})$ is not practicable. For example, evaluation of $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ could require the solution of a complex system of nonlinear partial differential equations as is the case for the BRAGFLO model in Table 2. Typically, a sampling-based approach is used to approximate $prob(c > C|\mathbf{x}_{st})$. For example, a random sample $\mathbf{x}_{su,i}$, $i = 1, 2, \ldots, nS$, generated in consistency with the definition of $(S_{su}, \mathcal{A}_{su}, p_{su})$ (i.e., in practice, in consistency with the distributions in Eq. (20) and any associated restrictions) leads to the approximation

$$prob(c > C \mid \mathbf{x}_{st}) \doteq \sum_{i=1}^{nS} \delta_C[f(\mathbf{x}_{st}, \mathbf{x}_{su,i})]/nS. \tag{23}$$

The resultant approximation is similar in appearance to that shown in Fig. 2 except that $C = f(\mathbf{x}_{st}, \mathbf{x}_{su,i})$ appears on the abscissa and $prob(c > C|\mathbf{x}_{st})$ appears on the ordinate.

The probability space $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ leads to distributions of CCDFs resulting from stochastic uncertainty as indicated in Fig. 3. When viewed formally, such distributions are defined by double integrals involving $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$, f, and $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$. The formal notation for such integrals is messy[45] and will not be presented here.

As previously indicated, integrals involving $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ and f are often evaluated with numerical procedures based on random sampling or importance sampling. Integrals involving $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ are often evaluated with procedures based on Latin hypercube sampling[46, 47] because of its efficient stratification properties. In particular, Latin hypercube sampling shows less sampling variability than simple random sampling[46, 48, 49] and has been observed to produce stable results in several large analyses.[50-52]

Latin hypercube sampling operates in the following manner to generate a sample of size *nLHS* from *nV* variables. The range of each variable (i.e., the x_j in Eq. (18)) is divided into *nLHS* intervals of equal probability and one value is selected at random from each interval. The *nLHS* values thus obtained for x_1 are paired at random and without replacement with the *nLHS* values obtained for x_2. These *nLHS* pairs are paired at random and without replacement with the *nLHS* values of x_3 to form *nLHS* triples. This process is continued until a set of *nLHS nV*-tuples is formed. These *nV*-tuples are of the form

$$\mathbf{x}_{su,i} = [x_{1i}, x_{2i}, \ldots, x_{nV,i}], \; i = 1, \ldots, nLHS, \tag{24}$$

and constitute the Latin hypercube sample (LHS). The individual x_j must be independent for the preceding construction procedure to work; however, a method for generating LHSs from correlated variables has been developed by Iman and Conover.[53, 54] As illustrated in Fig. 4 for an LHS from two variables, Latin hypercube sampling results in a dense stratification across the range of each variable (i.e., there is one value from each equal probability interval).

In the 1996 WIPP PA, three replicated (i.e., independently generated) LHSs of size *nLHS* = 100 from the variables indicated in Eq. (21) and Table 3 were used.[56] Further, the Iman/Conover restricted pairing technique[53, 54] was used to induce specified rank correlations between certain pairs of variables and also to ensure that all other pairs of variables had rank correlations close to zero. Each replicated sample was of the form

$$\mathbf{x}_{su,i} = [x_{1i}, x_{2i}, \ldots, x_{57,i}], \; i = 1, 2, \ldots, nLHS = 100, \tag{25}$$

and pooling all three replicates (designated R1, R2, R3) resulted in a single sample of size 300. Replicated sampling provided a way to observe the stability of results obtained with Latin hypercube sampling. Specifically, it was possible to determine if similar results were obtained with the individual samples, which did indeed turn out to be the case. As a reminder, Latin hypercube sampling is being used to implement a numerical integration, and so it is the stability of this numerical integration that is being investigated with the replicated samples.

Once the LHS is generated, PA results are calculated for each sample element. For EN2 and individual futures $\mathbf{x}_{st}$, this creates a mapping

$$[\mathbf{x}_{su,i}, \mathbf{f}(\mathbf{x}_{st}, \mathbf{x}_{su,i})], \; i = 1, 2, \ldots, nLHS, \tag{26}$$

from uncertain inputs to results for specific futures. Typically, a relatively small number of futures is selected for detailed analysis of this type (e.g., 5 - 10). As a reminder, $\mathbf{f}$ is usually quite complex and in practice is composed of many models (e.g., see Eq. (10) and Table 2). Further, all models represented by $\mathbf{f}$ may not be used in the analysis of all futures selected for consideration. In particular, different models or suites of models might be used to analyse different futures at the facility under consideration or to calculate different outcomes of interest for a given future. As an example, the individual model calculations performed in the 1996 WIPP PA are indicated in Table 4.

For CCDFs, a mapping of the form

$$[\mathbf{x}_{su,i}, prob(c > C \mid \mathbf{x}_{su,i})], \; i = 1, 2, \ldots, nLHS, \tag{27}$$

is created, where $prob(c > C \mid \mathbf{x}_{su,i})]$ defines the CCDF for some consequence of interest as indicated in Eqs. (11) and (19) (i.e., a CCDF results when C is allowed to run across all possible values of the consequence). In most PAs, CCDFs are generated for a large number of consequences.

The mappings in Eqs. (26) and (27) provide the basis for both uncertainty analysis and sensitivity analysis. Uncertainty analysis designates the determination of the uncertainty in analysis outcomes that results from uncertainty in analysis inputs. Specifically, uncertainty analysis involves the determination of the effects of the uncertainty characterized by EN3 and thus is providing an answer to question Q4 as indicated in Sect. 1. Once the calculations that lead to the mappings in Eqs. (26) and (27) are completed, the presentation of uncertainty analysis results simply involves the plotting of the predicted results with an equal weight (i.e., the reciprocal of the sample size) given to the individual results when either random or Latin hypercube sampling is used in the generation of the sample in Eq. (24). Sensitivity analysis designates the determination of the effects of individual variables contained in $\mathbf{x}_{su}$ on the observed uncertainty in predictions of interest. For sampling-based propagations of uncertainty, sensitivity analysis involves an exploration of the mappings in Eqs. (26) and (27) with techniques based on examination of scatterplots, correlation analysis, regression analysis, and the identification of nonrandom patterns.[57-59]

7. Example Results from PAs for the WIPP

7.1 Two-Phase Flow in Vicinity of Repository

The representation of two-phase flow in the vicinity of the repository in analyses for the WIPP is typical of the modeling problems encountered in a PA for a waste disposal site or some other facility. The model consists of three components: (i) a formal mathematical description of the model as a system of nonlinear partial differential equations (Sect. 4.2.1, Ref. 31), (ii) a numerical solution procedure based on finite difference techniques (Sect. 4.2.8, Ref. 31), and (iii) a computer program, BRAGFLO, that actually implements the numerical procedure and carries out various input and output processing activities (Ref. 60). For convenience, this model will be referred to as BRAGFLO although technically BRAGFLO is just the computer program that implements a particular numerical solution procedure for the model. As is typical of many programs, BRAGFLO can implement a variety of models through appropriate specification of input. The use of this model must be supported by the development of appropriate data (Sect. 4.2, Ref. 31; Refs. 61, 62). Further, there exists considerable uncertainty in many of the inputs used by the model (e.g., see Table 3). In the context of the entities EN1, EN2 and EN3 introduced in Sect. 1, the two-phase flow model is part of EN2, and the characterization of the uncertainty in the inputs used by this model is part of EN3.

Repository pressure under undisturbed conditions provides an example of the type of results calculated by BRAGFLO (Fig. 5a), with each curve resulting from a single calculation for one of the LHS elements associated with replicate R1 (see Eq. (25)). The spread of the curves is resulting from subjective uncertainty and is thus providing a representation of state of knowledge uncertainty with respect to predicted pressure in the repository.

As Fig. 5a contains results for 100 LHS elements, its generation required solution of the underlying system of nonlinear partial differential equations 100 times. Thus, the numerical algorithm in use must be sufficiently efficient to allow this number of calculations. Further, the algorithm must also be reasonably robust in the sense of not requiring large amounts of analyst intervention to produce a suitably converged solution. Such intervention is acceptable for a few solutions but would result in unacceptable requirements for analyst time if it was required for a large number of solutions.

Sensitivity analysis provides a way to determine which of the uncertain components of $\mathbf{x}_{su}$ are actually giving rise to the uncertainty in pressure shown in Fig. 5a. One way to make this determination is by calculating partial rank correlation coefficients (PRCCs) between the elements of $\mathbf{x}_{su}$ and the pressures above individual times on the abscissa of Fig. 5a. The resultant PRCCs can then be plotted to produce a time-dependent display of variable importance (Fig. 5b). As indicated in Fig. 5b, the uncertainty in pressure is dominated by the inputs *WMICDFLG*, *WGRCOR*, *WASTWICK* and *HALPOR*, with pressure tending to increase as each of these variables increases. Many additional techniques for sensitivity analysis are also available.[57-59]

As described in conjunction with Eqs. (22) and (23), the uncertainty associated with $\mathbf{x}_{su}$ leads to a distribution of possible analysis outcomes. For time-dependent repository pressure, this distribution is in essence shown by a plot of the resultant pressure curves (Fig. 5a). The more formal representation associated with Eqs. (22) and (23) can be calculated for individual times on the abscissa of Fig. 5a (e.g., at 10,000 yr as illustrated in Fig. 6). The curve labeled CCDF in Fig. 6 corresponds to a plot of the approximation to $prob(c > C|\mathbf{x}_{st})$ defined in Eq. (23), with the consequence associated with c and C corresponding to repository pressure at 10,000 yr, the future $\mathbf{x}_{st}$ corresponding to undisturbed conditions (i.e., no human disruption of the repository), and the summation taken over the $nS = 300$ LHS elements that result from pooling replicates R1, R2 and R3 (see Eq. (25)).

The results summarized in Fig. 6 are for pressure at a single time (i.e., 10,000 yr). For results of the form in Fig. 5a, selected quantiles (e.g., 0.10, 0.50, 0.90) and also the expected value can be calculated at selected times on the abscissa and then connected to form curves that present quantiles and means as a function of time (Fig. 7). The indicated calculations involve evaluating the results in Fig. 6 at a sequence of times. The results in Fig. 7 actually involve three sets of curves, with each set having been generated from one of the three replicated LHSs of size $nLHS = 100$ each (see Eq. (25)). The purpose of replicating the LHSs was to assess the stability of the associated integration over the probability space ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}) in the 1996 WIPP PA. As the closeness of the individual curves in Fig. 7 shows, the pressure results obtained with an LHS of size 100 were quite stable. Indeed, there were no cases in the 1996 WIPP PA when the individual replicates would have lead to different assessments of the potential behavior of the site.

7.2 Construction of CCDFs

As discussed in conjunction with Eqs. (11), (12) and (14), construction of CCDFs resulting from stochastic (i.e., aleatory) uncertainty can be viewed as a numerical integration problem involving the probability space ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) and models that predict the analysis result under consideration. Thus, construction of a CCDF involves both EN1 and EN2. Further, as discussed in conjunction with Eq. (19), different values for the uncertain input $\mathbf{x}_{su}$ lead to different CCDFs, with a distribution of CCDFs resulting from the probability space ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}) that corresponds to the entity E3.

Although a number of different release pathways to the accessible environment were considered in the 1996 WIPP PA, only the direct release pathways (i.e., cuttings and cavings, spallings, and direct brine release) produced nonzero releases. As a result, the function f in Eq. (10) reduces to

$$f(\mathbf{x}_{st}) = f_C(\mathbf{x}_{st}) + f_{SP}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})] + f_{DBR}\{\mathbf{x}_{st}, f_{SP}[\mathbf{x}_{st}, \mathbf{f}_B(\mathbf{x}_{st})], \mathbf{f}_B(\mathbf{x}_{st})\}, \tag{28}$$

and CCDFs were constructed for f_C, f_{SP}, f_{DBR} and the total release f (Fig. 8). As discussed in Sect. 5, the individual CCDFs resulted from a numerical integration over ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) based on Monte Carlo procedures. Further, the

multiple CCDFs in each frame resulted from a numerical integration over ($\mathcal{S}_{su}$, $\mathcal{J}_{su}$, p_{su}) based on Latin hypercube sampling (see Eq. (25)).

The primary regulatory requirement placed on the WIPP is that the CCDF for total release to the accessible environment (Fig. 8d) fall below the boundary line designated "EPA Limit" in Fig. 8 (p. 38086, Ref. 63). Further, an additional regulation specifies that the uncertainty in the value of this CCDF is to be determined and presented (pp. 5242-5243, Ref. 19). As examination of Fig. 8 shows, the CCDFs fall below the EPA limit when the effects of subjective uncertainty are assessed and propagated through the analysis. The EPA limit appearing in Fig. 8 is an example of what is sometimes called the Farmer limit line approach to the definition of acceptable risk.[64-67]

Mean and quantile curves were used to summarize the distribution of pressure curves (Figs. 5a, 7). A similar summary can be used for a distribution of CCDFs and provides a more quantitative summary of where the CCDF under consideration is believed to be located than is obtained from a visual examination of the corresponding distribution of CCDFs (Fig. 9). Formally, the results in Fig. 9 can be represented as a double integral involving ($\mathcal{S}_{st}$, $\mathcal{J}_{st}$, p_{st}) and ($\mathcal{S}_{su}$, $\mathcal{J}_{su}$, p_{su}), with these results being approximated with procedures based on random sampling and Latin hypercube sampling as previously described.

The replicated LHSs discussed in conjunction with Eq. (25) can also be used to examine the stability of the estimated CCDF distributions. The least stable estimates were obtained for the direct brine releases (Fig. 10). However, even in this case, the numerical variability in the estimated distribution is unimportant given the wide removal of the distribution from the EPA limit. The estimates for the other CCDF distributions were very stable, with the individual replicates producing mean and quantile curves that were almost indistinguishable.

8. Summary

A PA for a radioactive waste disposal site or some other facility is a complex mathematical calculation. In such a calculation, it is important to have a clear view of both the formal mathematical components on which the PA is based and the numerical procedures used in the approximation of these components. Appropriate numerical procedures and software that implements these procedures are essential parts of a PA. However, it is also important to maintain the conceptual distinction between a mathematical model and the numerical procedures used to implement that model.

Significant uncertainties exist in most PAs. Failure to acknowledge and represent this uncertainty can result in serious criticism of a PA. Indeed, a PA that does not provide a representation of the uncertainty in its outcomes is incomplete. As discussed, most PAs involve both stochastic (i.e., aleatory) and subjective (i.e., epistemic) uncertainty. The incorporation of uncertainty into a PA is essentially a multidimensional integration problem and

can place significant computational burdens on the analysis. Again, good numerical procedures and appropriate computational strategies are essential.

The resolution required in both models and numerical procedures is influenced by the uncertainty associated with the data that underlie a PA. Ultimately, the quality of model predictions is constrained by the quality of both the models in use and the available data to support these models. Although erroneous or nonconverged numerical procedures produce results of no value, acceptable errors in appropriately operating numerical procedures are, to some extent, determined by the uncertainty in model predictions that results from lack of resolution in the model or uncertainty in its inputs. Uncertainty and sensitivity analyses are important components of a PA and help provide guidance on both the uncertainty in outcomes of interest and where to best invest additional effort to reduce this uncertainty.

The modeling of physical processes is often done on two levels in a PA. First, very detailed models are used to develop and demonstrate an understanding of particular processes. Such models are often conceptually complex and numerically demanding and help identify the essential physical processes that must be considered in the final, integrative calculations of the PA. Second, less detailed models that embody the essential processes identified in prior analyses are often used in the final, integrative calculation. These models are less computationally intensive and serve to incorporate information gained from the more detailed models and other sources into the PA.

Reducing computational cost through the use of good numerical procedures and appropriate computational strategies is an important part of any large PA. Designing the PA in a way that will facilitate its implementation, documentation and review is also an important consideration. In most PAs, the cost of the human time to implement, document and review the analysis is much greater than the cost of the computation itself.

Quality documentation is an essential part of a successful PA. Such documentation requires a clear conceptual understanding of the PA and the role that various numerical procedures play in the computational implementation of the PA. Most PAs understand the time and resources required to produce adequate documentation. Yet, without such documentation, much of the value of a PA is lost.

Performance assessment should be an iterative process and should be initiated early in the analysis of a particular site or facility. Initially, PA can be primarily exploratory and relatively simple. Early PA efforts provide opportunities for (i) interactions between experimentalists and modelers, (ii) uncertainty and sensitivity analysis, (iii) development of insights with respect to the systems under study, (iv) outside review, (v) regulator and stakeholder involvement, (vi) initiation of a Quality Assurance (QA) program, and (vii) education of analysis participants on what to expect in later analyses. From such efforts, guidance emerges on (i) experimental programs and data development, (ii) model development, including the appropriateness of more or less complex models, and (iii) computational structure for a fully integrated analysis.

Intermediate PAs are typically more complex than initial PAs. At times, intermediate PAs are pushed towards unnecessary complexity or complexity that exceeds available data by model developers or outside reviewers. However, PAs tend to improve through multiple iterations as (i) more data becomes available or increased understanding improves the match between available data and model requirements, (ii) the appropriateness and implementation of individual models improves, (iii) the design and assembly of the entire PA improves due to increased understanding of both the overall system and results obtained from individual models, and (iv) the benefits of an appropriately implemented QA program are realized. In addition, continued iterations provide opportunities for (i) review of alternative models, (ii) uncertainty and sensitivity analysis, (iii) identification of errors in analysis or model implementation, and (iv) continued education of analysis participants, regulators, and stakeholders.

The final PA (e.g., a PA supporting a regulatory decision) benefits from the experiences of the prior analyses, including (i) a well-defined and well-tested analysis system that will produce no surprises in the final analysis, (ii) an analysis focused on recognized needs and requirements, (iii) use of models appropriate for the requirements of the analysis, including use of simplified models when prior analyses have indicated that this is acceptable due to either analysis requirements or resolution in available data, (iv) QA procedures emplaced and employed with models and an analysis system that have been previously used and tested, and (v) analysts, reviewers, regulators and stakeholders who are familiar with the analysis due to prior involvement.

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References

1. Rechard, R.P. 1999. "Historical Relationship Between Performance Assessment for Radioactive Waste Disposal and Other Types of Risk Assessment in the United States," *Risk Analysis*. Vol. 19, no. 5, pp. 763-807.

2. Thompson, B.G.J. 1999. "The Role of Performance Assessment in the Regulation of Underground Disposal of Radioactive Wastes: An International Perspective," *Risk Analysis*. Vol. 19, no. 5, pp. 809-846.

3. Gallegos, D.P. and E.J. Bonano. 1993. "Consideration of Uncertainty in the Performance Assessment of Radioactive Waste Disposal from an International Regulatory Perspective," *Reliability Engineering and System Safety*. Vol. 42, no. 2-3, pp. 111-123.

4. Thompson, B.G.J. and B. Sagar. 1993. "The Development and Application of Integrated Procedures for Post-Closure Assessment, Based Upon Monte Carlo Simulation: The Probabilistic Systems Assessment (PSA) Approach," *Reliability Engineering and System Safety*. Vol. 42, no. 2-3, pp. 125-160.

5. Helton, J.C., D.R. Anderson, H.-N. Jow, M.G. Marietta, and G. Basabilvazo. 1999. "Performance Assessment in Support of the 1996 Compliance Certification Application for the Waste Isolation Pilot Plant," *Risk Analysis*. Vol. 19, no. 5, pp. 959 - 986.

6. NRC (National Research Council). 1996. *The Waste Isolation Pilot Plant: A Potential Solution for the Disposal of Transuranic Waste*. Washington, DC: National Academy Press.

7. U.S. DOE (U.S. Department of Energy). 1998. *Viability Assessment of a Repository at Yucca Mountain*, DOE/RW-0508. Vols. 1-5. Las Vegas, NV: U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

8. Atomic Energy of Canada Limited. 1994. *Summary of the Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste*, AECL-10721; COG-93-11. Pinawa, Manitoba, Canada: Atomic Energy of Canada Limited, Whiteshell Nuclear Research Establishment.

9. Swedish Nuclear Power Inspectorate. 1996. *SKI SITE-94. Deep Repository Performance Assessment Project*, SKI Report 96:36. Stockholm, Sweden: Swedish Nuclear Power Inspectorate.

10. Hoorelbeke, J.M. and B. Mouroux. 1998. "Design and Safety Assessment of Geological Assessment - Development Plan," *Proceedings, DISTIC '98, Disposal Technologies and Concepts 1998, International Conference on Radioactive Waste Disposal, September 9-11, 1998, Hamburg*. Ed. A. Roth. Hamburg, Germany: Kontec Gesellshaft für Technische Kommunication. pp. 216-221.

11. Helton, J.C. 1997. "Uncertainty and Sensitivity Analysis in the Presence of Stochastic and Subjective Uncertainty," *Journal of Statistical Computation and Simulation*. Vol. 57, no. 1-4, pp. 3-76.

12. Helton, J.C. and D.E. Burmaster. 1996. "Guest Editorial: Treatment of Aleatory and Epistemic Uncertainty in Performance Assessments for Complex Systems," *Reliability Engineering and System Safety*. Vol. 54, no. 2-3, pp. 91-94.

13. Paté-Cornell, M.E. 1996. "Uncertainties in Risk Analysis: Six Levels of Treatment," *Reliability Engineering and System Safety*. Vol. 54, no. 2-3, pp. 95-111.

14. Thompson, K.M. and J.D. Graham. 1996. "Going Beyond the Single Number: Using Probabilistic Risk Assessment to Improve Risk Management," *Human and Ecological Risk Assessment*. Vol. 2, no. 4, pp. 1008-1034.

15. Helton, J.C. 1994. "Treatment of Uncertainty in Performance Assessments for Complex Systems," *Risk Analysis*. Vol. 14, no. 4, pp. 483-511.

16. Hoffman, F.O. and J.S. Hammonds. 1994. "Propagation of Uncertainty in Risk Assessments: The Need to Distinguish Between Uncertainty Due to Lack of Knowledge and Uncertainty Due to Variability," *Risk Analysis*. Vol. 14, no. 5, pp. 707-712.

17. Bernstein, P.L. 1996. *Against the Gods: The Remarkable Story of Risk*. New York, NY: John Wiley & Sons, Inc.

18. Hacking, I. 1975. *The Emergence of Probability: A Philosophical Study of Early Ideas About Probability, Induction and Statistical Inference*. New York, NY; London, England: Cambridge University Press.

19. U.S. EPA (U.S. Environmental Protection Agency). 1996. "40 CFR Part 194: Criteria for the Certification and Re-Certification of the Waste Isolation Pilot Plant's Compliance With the 40 CFR Part 191 Disposal Regulations; Final Rule," *Federal Register*. Vol. 61, no. 28, pp. 5224-5245.

20. Stenhouse, M., N. Chapman, and T. Sumerling. 1993. *SITE-94 Scenario Development FEP Audit List Preparation: Methodology and Presentation*, SKI Technical Report 93:27. Stockholm, Sweden: Swedish Nuclear Power Inspectorate.

21. Goodwin, B.W., M.E. Stephens, C.C. Davison, L.H. Johnson, and R. Zach. 1994. *Scenario Analysis for the Postclosure Assessment of the Canadian Concept for Nuclear Fuel Waste Disposal*, AECL-10969, COG94-247. Pinawa, Manitoba, Canada: Atomic Energy of Canada Ltd., Whiteshell Laboratories.

22. Andersson, J. (ed.), T. Carlsson, T. Eng. F. Kautsky, E. Söderman, and S. Wingefors. 1989. *The Joint SKI/SKB Scenario Development Project*, SKB Technical Report 89-35. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Co.

23. NAGRA. 1985. *Nuclear Waste Management in Switzerland: Feasibility Studies and Safety Analyses (Project Gewahr, 1985)*, NAGRA Project Report NGB 85-09 (English Summary). Wettingen, Switzerland: National Cooperative for the Storage of Radioactive Waste.

24. Thorne, M.C. 1993. "The Use of Expert Opinion in Formulating Conceptual Models of Underground Disposal Systems and the Treatment of Associated Bias," *Reliability Engineering and System Safety*. Vol. 42, no. 2-3, pp. 161-180.

25. Miller, W.M. and N.A. Chapman, Ed. 1992. *Identification of Relevant Processes, System Concept Group Report*, UKDOE/HMIP Report TR-ZI-11. London, England: Environment Agency.

26. Hodgkinson, D.P. and T.J. Sumerling. 1989. "A Review of Approaches to Scenario Analysis for Repository Safety Assessment," *Proceedings of the IAEA/CEC/NEA (OECD) Symposium on Safety Assessment of Radioactive Waste Repositories*. Paris, France: Organisation for Economic Co-operation and Development. pp. 333-350.

27. Cranwell, R.M., R.V. Guzowski, J.E. Campbell, and N.R. Ortiz. 1990. *Risk Methodology for Geologic Disposal of Radioactive Waste: Scenario Selection Procedure*, NUREG/CR-1667, SAND80-1429. Albuquerque, NM: Sandia National Laboratories.

28. U.S. DOE (U.S. Department of Energy). 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant*, DOE/CAO-1996-2184. Vols. I-XXI. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.

29. U.S. EPA (U.S. Environmental Protection Agency). 1993. "40 CFR 191: Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes; Final Rule," *Federal Register*. Vol. 58, no. 242, pp. 66398-66416.

30. Feller, W. 1971. *An Introduction to Probability Theory and Its Applications*. Vol. II. 2nd ed. New York, NY: John Wiley & Sons.

31. Helton, J.C., J.E. Bean, J.W. Berglund, F.J. Davis, K. Economy, J.W. Garner, J.D. Johnson, R.J. MacKinnon, J. Miller, D.G. O'Brien, J.L. Ramsey, J.D. Schreiber, A. Shinta, L.N. Smith, D.M. Stoelzel, C. Stockman, and P. Vaughn. 1998. *Uncertainty and Sensitivity Analysis Results Obtained in the 1996*

Performance Assessment for the Waste Isolation Pilot Plant, SAND98-0365. Albuquerque, NM: Sandia National Laboratories.

32. Press, W.H., S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery. 1992. *Numerical Recipes in Fortran: The Art of Scientific Computing*. 2nd ed. Cambridge, England; New York, NY: Cambridge University Press.

33. Helton, J.C., J.D. Johnson, H.-N. Jow, R.D. McCurley, and L.J. Rahal. 1998. "Stochastic and Subjective Uncertainty in the Assessment of Radiation Exposure at the Waste Isolation Pilot Plant," *Human and Ecological Risk Assessment*. Vol. 4, no. 2, pp. 469-526.

34. Sokolnikoff, I.S. and R.M. Redheffer. 1966. *Mathematics of Physics and Modern Engineering*. 2nd ed. New York, NY: McGraw-Hill Book Co.

35. Breeding, R.J., J.C. Helton, E.D. Gorham, and F.T. Harper. 1992. "Summary Description of the Methods Used in the Probabilistic Risk Assessments for NUREG-1150," *Nuclear Engineering and Design*. Vol. 135, no. 1, pp. 1-27.

36. Vesely, W.E., F.F. Goldberg, N.H. Roberts, and D.F. Haasl. 1981. *Fault Tree Handbook*, NUREG-0492. Washington, DC: U.S. Nuclear Regulatory Commission.

37. Helton, J.C. and H.J. Iuzzolino. 1993. "Construction of Complementary Cumulative Distribution Functions for Comparison with the EPA Release Limits for Radioactive Waste Disposal," *Reliability Engineering and System Safety*. Vol. 40, no. 3, pp. 277-293.

38. Bonano, E.J. and G.E. Apostolakis. 1991. "Theoretical Foundations and Practical Issues for Using Expert Judgments in Uncertainty Analysis of High-Level Radioactive Waste Disposal," *Radioactive Waste Management and the Nuclear Fuel Cycle*. Vol. 16, no. 2, pp. 137-159.

39. Cooke, R.M. 1991. *Experts in Uncertainty: Opinion and Subjective Probability in Science*. Oxford, England: Oxford University Press.

40. Keeney, R.L. and D. von Winterfeldt. 1991. "Eliciting Probabilities from Experts in Complex Technical Problems," *IEEE Transactions on Engineering Management*. Vol. 38, no. 3, pp. 191-201.

41. Meyer, M.A. and J.M. Booker. 1991. *Eliciting and Analyzing Expert Judgment: A Practical Guide*. New York, NY: Academic Press.

42. Hora, S.C. and R.L. Iman. 1989. "Expert Opinion in Risk Analysis: The NUREG-1150 Methodology," *Nuclear Science and Engineering*. Vol. 102, no. 4, pp. 323-331.

43. Mosleh, A., V.M. Bier, and G. Apostolakis. 1988. "A Critique of Current Practice for the Use of Expert Opinions in Probabilistic Risk Assessments," *Reliability Engineering and System Safety*. Vol. 20, no. 1, pp. 63-85.

44. MacKinnon, R.J. and G. Freeze. 1997. "Summary of EPA-Mandated Performance Assessment Verification Test (Replicate 1) and Comparison with the Compliance Certification Application Calculations," Technical Data Package. Sandia WIPP Central Files WPO # 46674. Albuquerque, NM: Sandia National Laboratories.

45. Helton, J.C. 1996. "Probability, Conditional Probability and Complementary Cumulative Distribution Functions in Performance Assessment for Radioactive Waste Disposal," *Reliability Engineering and System Safety*. Vol. 54, no. 2-3, pp. 145-163.

46. McKay, M.D., R.J. Beckman, and W.J. Conover. 1979. "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code," *Technometrics*. Vol. 21, no. 2, pp. 239-245.

47. Iman, R.L. 1992. "Uncertainty and Sensitivity Analysis for Computer Modeling Applications," *Reliability Technology - 1992, The Winter Annual Meeting of the American Society of Mechanical Engineers, Anaheim, California, November 8-13, 1992*. AD-Vol. 28, Ed. T.A. Cruse. New York, NY: The American Society of Mechanical Engineers, Aerospace Division. pp. 153-168.

48. Stein, M. 1987. "Large Sample Properties of Simulations Using Latin Hypercube Sampling," *Technometrics*. Vol. 29, no. 2, pp. 143-151.

49. Owen, A.B. 1992. "A Central Limit Theorem for Latin Hypercube Sampling," *Journal of the Royal Statistical Society. Series B. Methodological*. Vol. 54, no. 2, pp. 541-551.

50. Iman, R.L. and J.C. Helton. 1988. "An Investigation of Uncertainty and Sensitivity Analysis Techniques for Computer Models," *Risk Analysis*. Vol. 8, no. 1, pp. 71-90.

51. Iman, R.L. and J.C. Helton. 1991. "The Repeatability of Uncertainty and Sensitivity Analyses for Complex Probabilistic Risk Assessments," *Risk Analysis*. Vol. 11, no. 4, pp. 591-606.

52. Helton, J.C., J.D. Johnson, M.D. McKay, A.W. Shiver, and J.L. Sprung. 1995. "Robustness of an Uncertainty and Sensitivity Analysis of Early Exposure Results with the MACCS Reactor Accident Consequence Model," *Reliability Engineering and System Safety*. Vol. 48, no. 2, pp. 129-148.

53. Iman, R.L. and W.J. Conover. 1982. "A Distribution-Free Approach to Inducing Rank Correlation Among Input Variables," *Communications in Statistics: Simulation and Computation*. Vol. B11, no. 3, pp. 311-334.

54. Iman, R.L. and J.M. Davenport. 1982. "Rank Correlation Plots for Use with Correlated Input Variables," *Communications in Statistics: Simulation and Computation*. Vol. B11, no. 3, pp. 335-360.

55. Helton, J.C. 1999. "Uncertainty and Sensitivity Analysis in Performance Assessment for the Waste Isolation Pilot Plant," *Computer Physics Communications*. Vol. 117, no. 1-2, pp. 156-180.

56. Iman, R.L. 1982. "Statistical Methods for Including Uncertainties Associated with the Geologic Isolation of Radioactive Waste Which Allow for a Comparison with Licensing Criteria," *Proceedings of the Symposium on Uncertainties Associated with the Regulation of the Geologic Disposal of High-Level Radioactive Waste, Gatlinburg, TN, March 9-13, 1981*. NUREG/CP-0022, CONF-810372. Eds. D.C. Kocher. Washington, DC: U.S. Nuclear Regulatory Commission, Directorate of Technical Information and Document Control. pp. 145-157.

57. Helton, J.C. 1993. "Uncertainty and Sensitivity Analysis Techniques for Use in Performance Assessment for Radioactive Waste Disposal," *Reliability Engineering & System Safety*. Vol. 42, no. 2-3, pp. 327-367.

58. Hamby, D.M. 1994. "A Review of Techniques for Parameter Sensitivity Analysis of Environmental Models," *Environmental Monitoring and Assessment*. Vol. 32, no. 2, pp. 125-154.

59. Kleijnen, J.P.C. and J.C. Helton. 1999. "Statistical Analyses of Scatterplots to Identify Important Factors in Large-Scale Simulations, 1: Review and Comparison of Techniques," *Reliability Engineering and System Safety*. Vol. 65, no. 2, pp. 147-185.

60. Schreiber, J.D. 1996. *BRAGFLO, Version 4.00 User's Manual*, Sandia WIPP Central Files WPO # 30703. Albuquerque, NM: Sandia National Laboratories

61. Larson, K.W. 2000. "Development of the Conceptual Models for Chemical Conditions and Hydrology Used in the 1996 Performance Assessment for the Waste Isolation Pilot Plant," *Reliability Engineering and System Safety*, to appear.

62. Bean, J.E., M.E. Lord, D.A. McArthur, R.J. MacKinnon, J.D. Miller, and J.D. Schreiber. 1996. "Analysis Package for the Salado Flow Calculations (Task 1) of the Performance Assessment Analysis Supporting the Compliance Certification Application (CCA)." Sandia WIPP Central Files WPO # 40514. Albuquerque, NM: Sandia National Laboratories.

63. U.S. EPA (U.S. Environmental Protection Agency). 1985. "40 CFR Part 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes; Final Rule," *Federal Register*. Vol. 50, no. 182, pp. 38066-38089.

64. Farmer, F.R. 1967. "Reactor Safety and Siting: A Proposed Risk Criterion," *Nuclear Safety*. Vol. 8, no. 6, pp. 539-548.

65. Cox, D.C. and P. Baybutt. 1982. "Limit Lines for Risk," *Nuclear Technology*. Vol. 57, no. 3, pp. 320-330.

66. Munera, H.A. and G. Yadigaroglu. 1986. "On Farmer's Line, Probability Density Functions, and Overall Risk," *Nuclear Technology*. Vol. 74, no. 2, pp. 229-232.

67. Helton, J.C. 1993. "Risk, Uncertainty in Risk, and the EPA Release Limits for Radioactive Waste Disposal," *Nuclear Technology*. Vol. 101, no. 1, pp. 18-39.

Figure Captions

Fig. 1. Example CCDF: plot of probability $prob(c > C)$ that a consequence with a value larger then C will occur.

Fig. 2. Approximation of a CCDF with a random sample of size 1000.

Fig. 3. Different values of CCDF defined by Eq. (11) that derive from different values of $\mathbf{x}_{su}$.

Fig. 4. Example of an LHS of size $nLHS = 10$ from variables U and V with U normal on [−1, 1] (mean = 0, 0.01 quantile = −1, 0.99 quantile = 1) and V triangular on [0, 4] (mode = 1) (Fig. 4, Ref. 55).

Fig. 5. Uncertainty and sensitivity analysis results for pressure (Pa) in waste panel under undisturbed (i.e., E0) conditions: (5a) time-dependent pressures for 100 LHS elements in replicate R1, and (5b) PRCCs obtained from analysis of all 300 LHS elements associated with replicates R1, R2 and R3 (Fig. 5, Ref. 55).

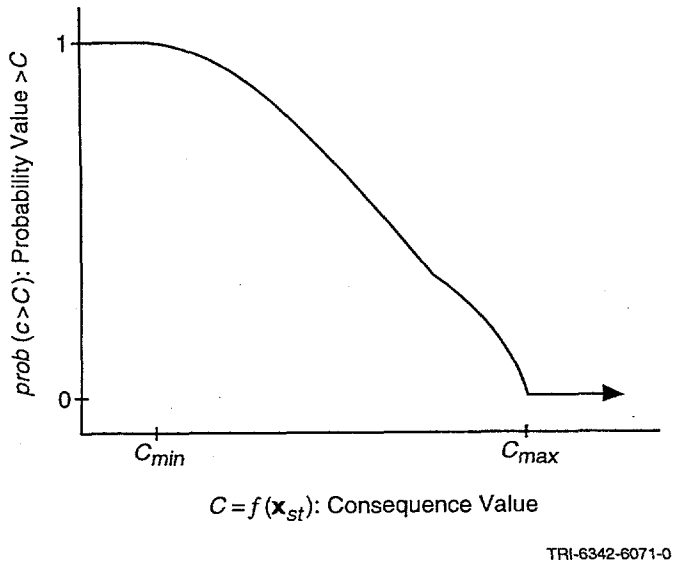
Fig. 6. Example of estimated CDF and CCDF for repository pressure at 10,000 yr under undisturbed conditions (i.e., $y = WAS\_PRES$) obtained from the 300 LHS elements that result from pooling replicates R1, R2 and R3 (see Eq. (25)).

Fig. 7. Mean and quantile curves for three replicated LHSs for pressure in lower waste panel under undisturbed conditions (Fig. 6, Ref. 55).

Fig. 8. Distributions of CCDFs resulting from subjective uncertainty and obtained with replicate R1 for the following release modes: (8a) cuttings and cavings, (8b) spallings, (8c) direct brine release, and (8d) total (i.e., cuttings and cavings, spallings, direct brine) (Figs. 6, 9, Ref. 33). The statements in Frames 8b and 8c that observations are offscale means that the largest normalized release for each of these observations is less than 10^{-5} EPA units, with the largest release for each of these observations typically being zero.

Fig. 9. Mean and quantile curves for distribution of total release CCDFs in Fig. 8d (Fig. 7, Ref. 33).

Fig. 10. Outcome of replicated sampling for distribution of CCDFs for normalized release to the accessible environment over 10,000 yr due to direct brine release (Fig. 12, Ref. 55).



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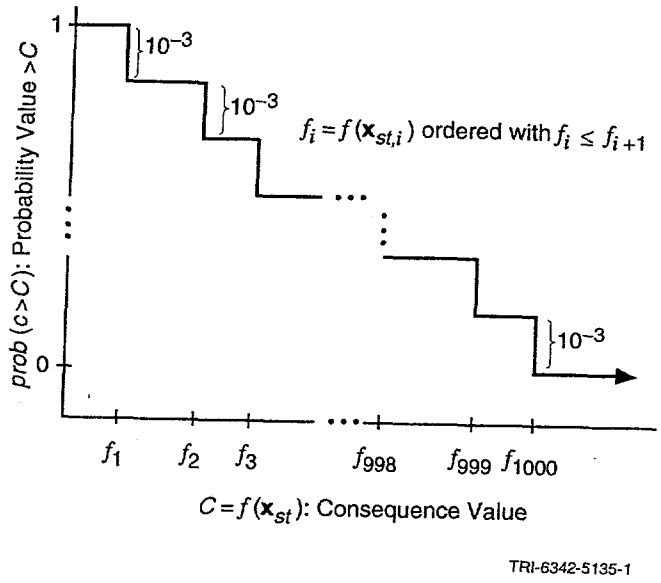

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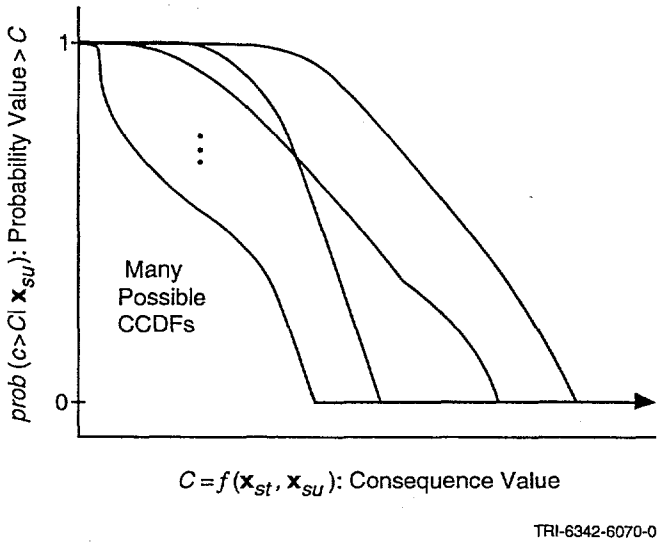

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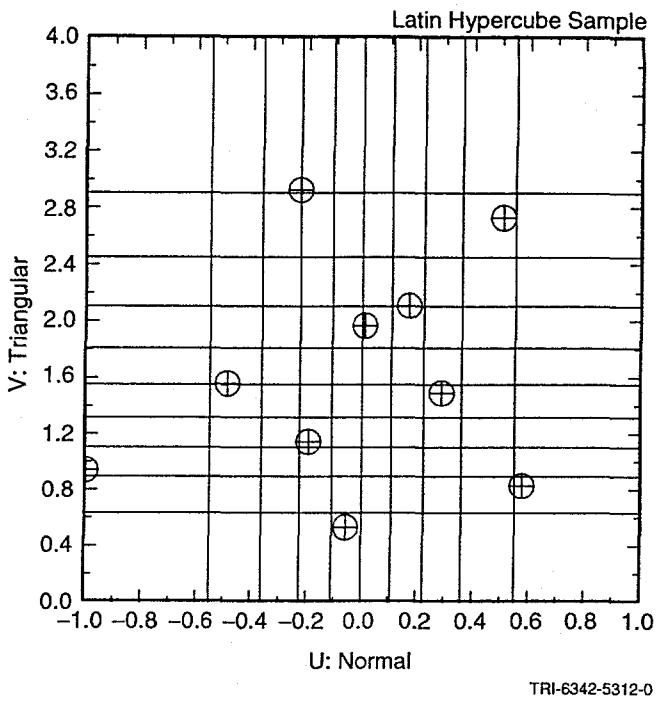

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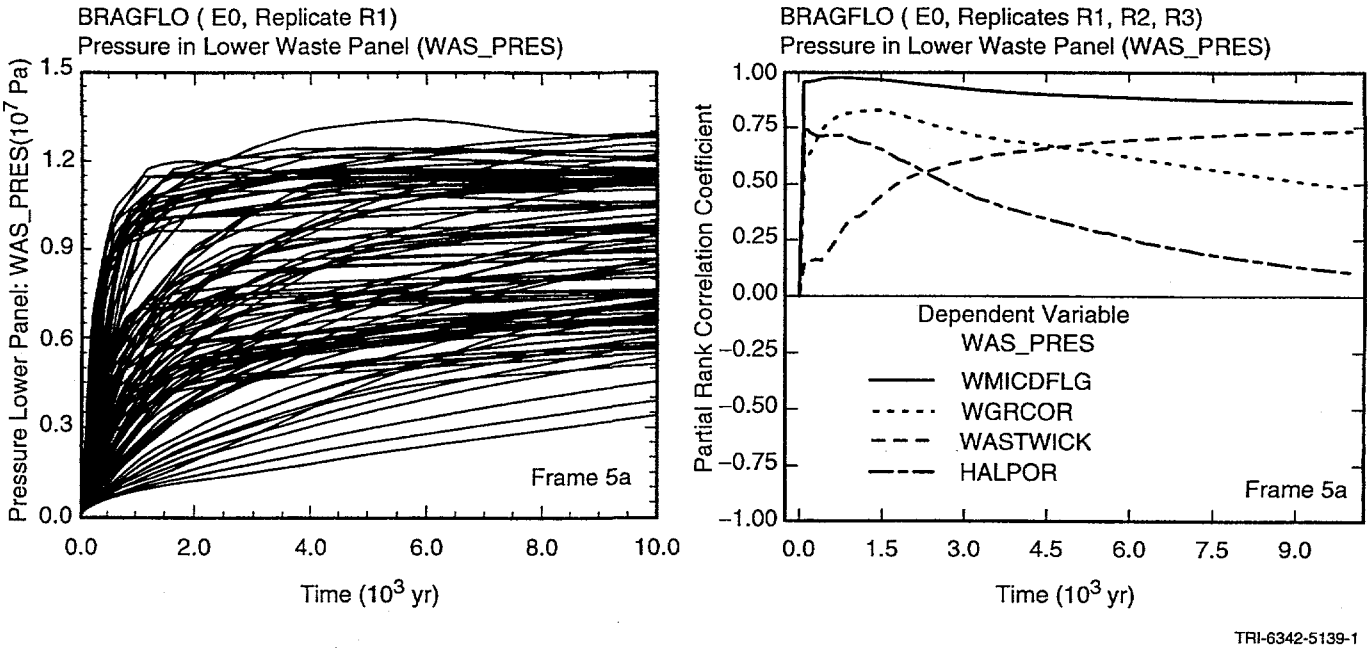

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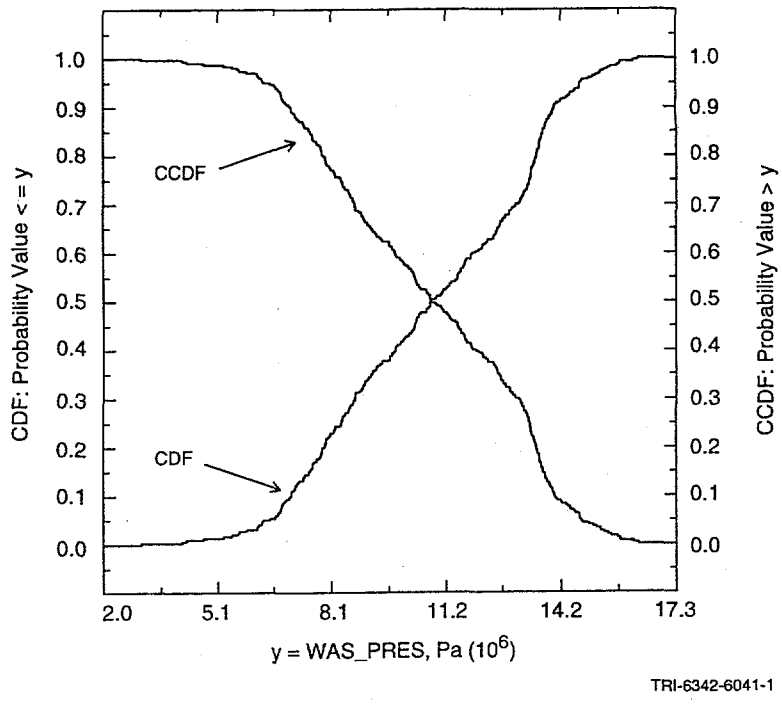

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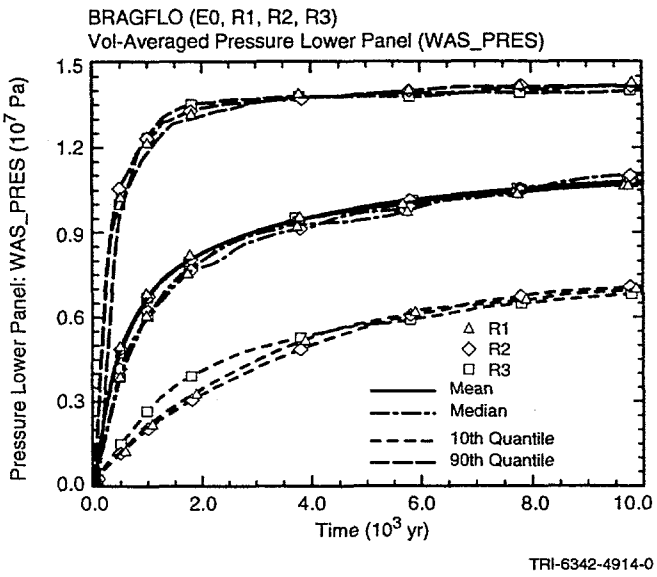

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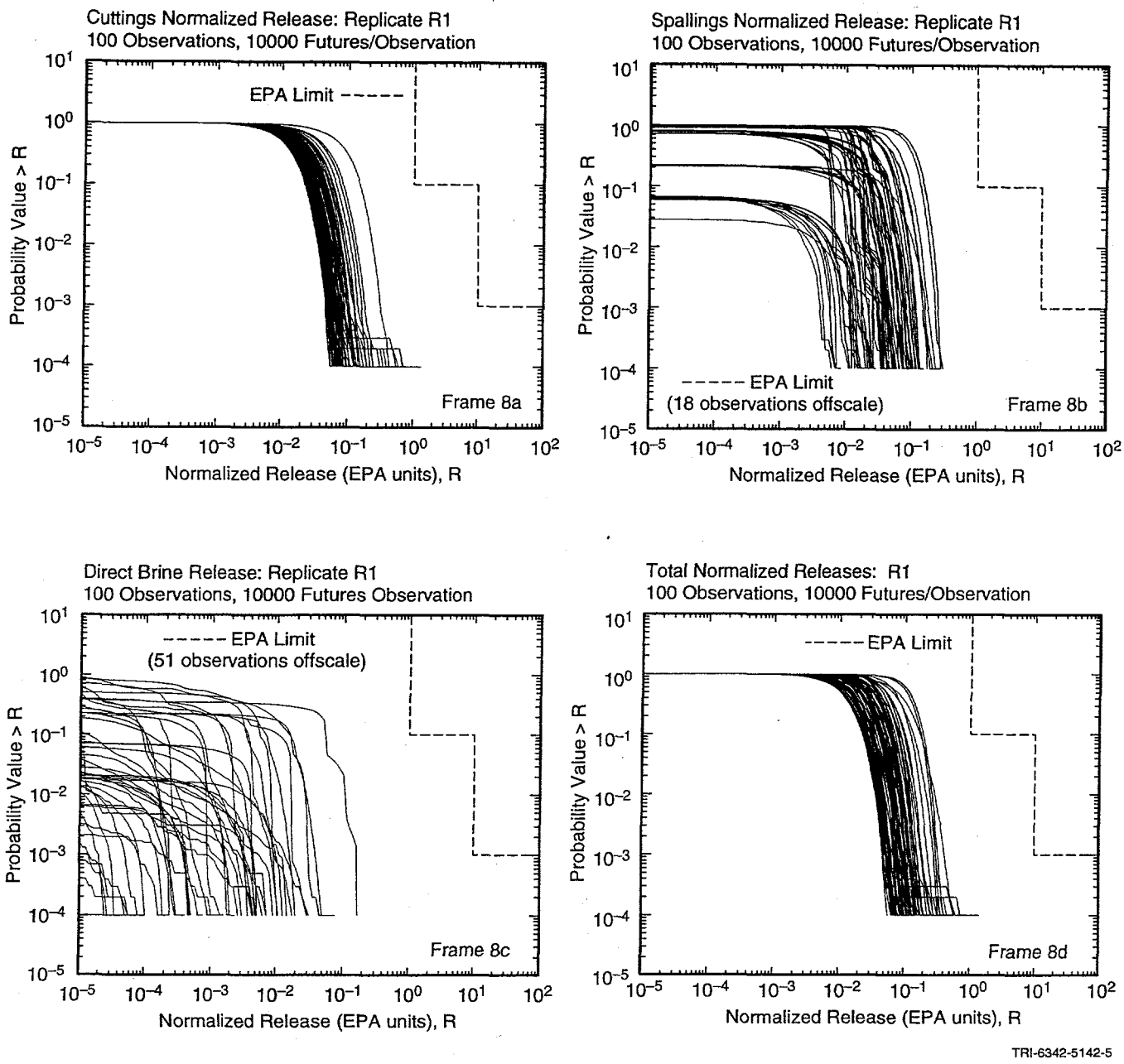

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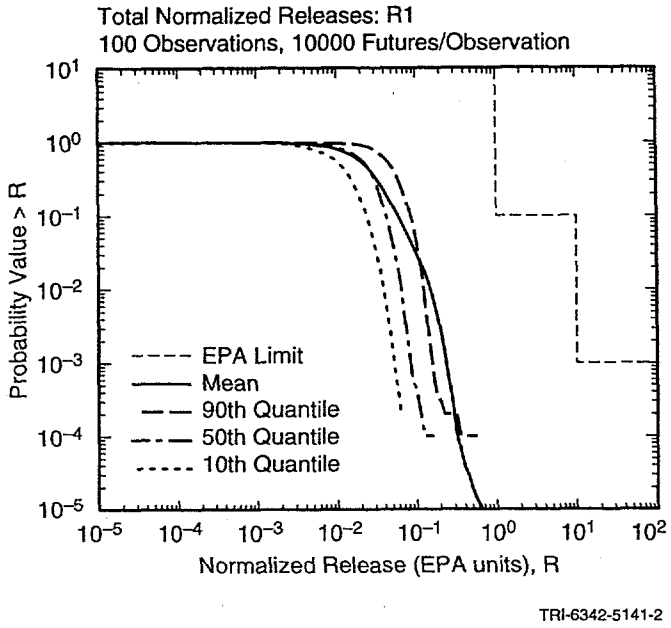

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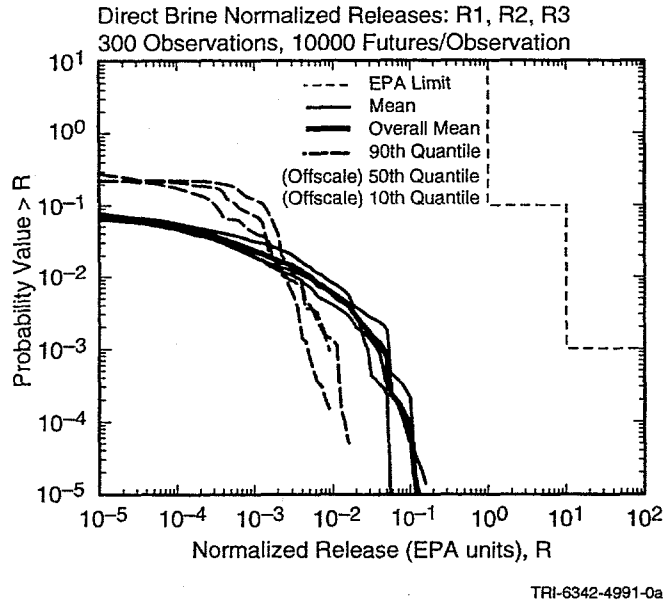

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Table 1. Natural FEPs and Their Screening Classifications (Table II, Ref. 5; adapted from Table 6-3, Ref. 28)

GEOLOGICAL FEPs (Sect. SCR.1.1, Ref. 28): 1. Stratigraphy. 1.1 Stratigraphy (UP). 1.2 Brine reservoirs (DP). 2. Tectonics. 2.1 Changes in regional stress (SO-C). 2.2 Regional tectonics (SO-C). 2.3 Regional uplift and subsidence (SO-C). 3. Structural FEPs. 3.1 Deformation. 3.1.1 Salt deformation (SO-P, UP near repository). 3.1.2 Diapirism (SO-P). 3.2 Fracture development. 3.2.1 Formation of fractures (SO-P, UP near repository). 3.2.2 Changes in fracture properties (SO-C, UP near repository). 3.3 Fault movement. 3.3.1 Formation of new faults (SO-P). 3.3.2 Fault movement (SO-P). 3.4 Seismic activity. 3.4.1 Seismic activity (UP). 4. Crustal processes. 4.1 Igneous activity. 4.1.1 Volcanic activity (SO-P). 4.1.2 Magmatic activity (SO-C). 4.2 Metamorphism. 4.2.1 Metamorphic activity (SO-P). 5. Geochemical FEPs. 5.1 Dissolution. 5.1.1 Shallow dissolution (UP). 5.1.2 Lateral dissolution (SO-C). 5.1.3 Deep dissolution (SO-P). 5.1.4 Solution chimneys (SO-P). 5.1.5 Breccia pipes (SO-P). 5.1.6 Collapse breccias (SO-P). 5.2 Mineralization. 5.2.1 Fracture infills (SO-C).

SUBSURFACE HYDROLOGICAL FEPs (Sect. SCR.1.2, Ref. 28): 1. Groundwater characteristics. 1.1 Saturated groundwater flow (UP). 1.2 Unsaturated groundwater flow (UP, SO-C in Culebra). 1.3 Fracture flow (UP). 1.4 Density effects on groundwater flow (SO-C). 1.5 Effects of preferential pathways (UP, UP in Salado and Culebra. 2. Changes in groundwater flow. 2.1 Thermal effects on groundwater flow (SO-C). 2.2 Saline intrusion (SO-P). 2.3 Freshwater intrusion (SO-P). 2.4 Hydrological response to earthquakes (SO-C). 2.5 Natural gas intrusion (SO-P).

SUBSURFACE GEOCHEMICAL FEPs (Sect. SCR.1.3, Ref. 28): 1. Groundwater geochemistry. 1.1 Groundwater geochemistry (UP). 2. Changes in groundwater chemistry. 2.1 Saline intrusion (SO-C). 2.2 Freshwater intrusion (SO-C). 2.3 Changes in groundwater Eh (SO-C). 2.4 Changes in groundwater pH (SO-C). 2.5 Effects of dissolution (SO-C).

GEOMORPHOLOGICAL FEPs (Sect. SCR.1.4, Ref. 28): 1. Physiography. 1.1 Physiography (UP). 2. Meteorite impact. 2.1 Impact of a large meteorite (SO-P). 3. Denudation. 3.1 Weathering. 3.1.1 Mechanical weathering (SO-C). 3.1.2 Chemical weathering. 3.2 Erosion. 3.2.1 Aeolian erosion (SO-C). 3.2.2 Fluvial erosion (SO-C). 3.2.3 Mass wasting (SO-C). 3.3 Sedimentation. 3.3.1 Aeolian deposition (SO-C). 3.3.2 Fluvial deposition (SO-C). 3.3.3 Lacustrine deposition (SO-C). 3.3.4 Mass Wasting (SO-C). 4. Soil development. 4.1 Soil development (SO-C).

SURFACE HYDROLOGICAL FEPs (Sect. SCR.1.5, Ref. 28): 1. Fluvial. 1.1 Stream and river flow (SO-C). 2. Lacustrine. 2.1 Surface water bodies (SO-C). 3. Groundwater recharge and discharge. 3.1 Groundwater discharge (UP). 3.2 Groundwater recharge (UP). 3.3 Infiltration (UP, UP for climate change effects). 4. Changes in surface hydrology. 4.1 Changes in groundwater recharge and discharge (UP). 4.2 Lake formation (SO-C). 4.3 River flooding (SO-C).

CLIMATIC FEPs (Sect. SCR.1.6, Ref. 28): 1. Climate. 1.1 Precipitation (for example, rainfall) (UP). 1.2 Temperature (UP). 2. Climate change. 2.1 Meteorological. 2.1.1 Climate change (UP). 2.2 Glaciation. 2.2.1 Glaciation (SO-P). 2.2.2 Permafrost (SO-P).

MARINE FEPs (Sect. SCR.1.7, Ref. 28): 1. Seas. 1.1 Seas and oceans (SO-C). 1.2 Estuaries (SO-C). 2. Marine sedimentology. 2.1 Coastal erosion (SO-C). 2.2 Marine sediment transport and deposition (SO-C). 3. Sea level changes. 3.1 Sea level changes (SO-C).

ECOLOGICAL FEPs (Sect. SCR.1.8, Ref. 28): 1. Flora and fauna. 1.1 Plants (SO-C). 1.2 Animals (SO-C). 1.3 Microbes (SO-C, UP for colloidal effects and gas generation). 2. Changes in flora and fauna. 2.1 Natural ecological development (SO-C).

Legend: UP ~ FEPs accounted for in the assessment calculations for undisturbed performance for 40 CFR § 191.13 (Ref. 29) (as well as 40 CFR § 191.15 and Subpart C of 40 CFR Part 191); DP ~ FEPs accounted for (in addition to all UP FEPs) in the assessment calculations for disturbed performance for 40 CFR § 191.13; SO-R ~ FEPs eliminated from PA calculations on the basis of regulations provided in 40 CFR Part 191 and criteria provided in 40 CFR Part 194 (Ref. 19); SO-C ~ FEPs eliminated from PA (and compliance assessment) calculations on the basis of consequence; SO-P ~ FEPs eliminated from PA (and compliance assessment) calculations on the basis of low probability of occurrence.

Table 2. Summary of Computer Models Used in the 1996 WIPP PA (adapted from Table I, Ref. 33, which can be consulted for sources of additional information)

BRAGFLO: Calculates multiphase flow of gas and brine through a porous, heterogeneous reservoir. Uses finite difference procedures to solve system of nonlinear partial differential equations that describes the mass conservation of gas and brine along with appropriate constraint equations, initial conditions and boundary conditions.

BRAGFLO_DBR: Special configuration of BRAGFLO model used in calculation of dissolved radionuclide releases to the surface (i.e., direct brine releases) at the time of a drilling intrusion. Uses initial value conditions obtained from calculations performed with BRAGFLO and CUTTINGS_S.

CUTTINGS_S: Calculates the quantity of radioactive material brought to the surface in cuttings and cavings and also in spallings generated by an exploratory borehole that penetrates a waste panel, where cuttings designates material removed by the drillbit, cavings designates material eroded into the borehole due to shear stresses resulting from the circular flow of the drilling fluid (i.e., mud), and spallings designates material carried to the borehole at the time of an intrusion due to the flow of gas from the repository to the borehole. Spallings calculation uses initial value conditions obtained from calculations performed with BRAGFLO.

GRASP-INV: Generates transmissivity fields (estimates of transmissivity values) conditioned on measured transmissivity values and calibrated to steady-state and transient pressure data at well locations using an adjoint sensitivity and pilot-point technique.

NUTS: Solves system of partial differential equations for radionuclide transport in vicinity of repository with finite difference procedures. Uses brine volumes and flows calculated by BRAGFLO as input.

PANEL: Calculates rate of discharge and cumulative discharge of radionuclides from a waste panel through an intruding borehole. Discharge is a function of fluid flow rate, elemental solubility and radionuclide inventory. Uses brine volumes and flows calculated by BRAGFLO as input. Based on closed-form solution of system of linear ordinary differential equations.

SANTOS: Solves quasistatic, large deformation, inelastic response of two-dimensional solids with finite element techniques. Used to determine porosity of waste as a function of time and cumulative gas generation, which is an input to calculations performed with BRAGFLO.

SECOFL2D: Calculates single-phase Darcy flow for groundwater flow in two dimensions. The formulation is based on a single partial differential equation for hydraulic head using fully implicit time differencing. Uses transmissivity fields generated by GRASP-INV.

SECOTP2D: Simulates transport of radionuclides in fractured porous media. Solves two partial differential equations: one provides two-dimensional representation for advective and diffusive radionuclide transport in fractures and the other provides one-dimensional representation for diffusion of radionuclides into rock matrix surrounding the fractures. Equations solved with finite difference procedures. Uses flow fields calculated by SECOFL2D.

Table 3. Example Elements of $\mathbf{x}_{su}$ in the 1996 WIPP PA (see App. PAR, Ref. 28, and Table 5.2.1, Ref. 31, for a complete listing of the nV = 57 elements of $\mathbf{x}_{su}$ and sources of additional information)

ANHPRM—Logarithm of anhydrite permeability (m^2). Used in BRAGFLO. Distribution: Student's t-distribution with 5 degrees of freedom. Range: –21.0 to –17.1 (i.e., permeability range is 1×10^{-21} to $1 \times 10^{-17.1}$ m^2). Mean, Median: –18.9, –18.9. Correlation : –0.99 rank correlation with *ANHCOMP* (Bulk compressibility of anhydrite, Pa^{-1}).

BHPRM—Logarithm of borehole permeability (m^2). Used in BRAGFLO. Distribution: Uniform. Range: –14 to –11 (i.e., permeability range is 1×10^{-14} to 1×10^{-11} m^2). Mean, median: –12.5, –12.5.

BPCOMP—Logarithm of bulk compressibility of brine pocket (Pa^{-1}). Used in BRAGFLO. Distribution: Triangular. Range: –11.3 to –8.00 (i.e., bulk compressibility range is $1 \times 10^{-11.3}$ to 1×10^{-8} Pa^{-1}). Mean, mode: –9.80, –10.0. Correlation: –0.75 rank correlation with *BPPRM* (Logarithm of brine pocket permeability, m^2).

BPINTPRS—Initial pressure in brine pocket (Pa). Used in BRAGFLO. Distribution: Triangular. Range: 1.11×10^7 to 1.70×10^7 Pa. Mean, mode: 1.36×10^7 Pa, 1.27×10^7 Pa.

CFRCSP—Culebra fracture spacing (m). Used in SECOTP2D. Equal to half the distance between fractures. Distribution: Uniform. Range: 0.05 to 0.5 m. Mean, median: 0.275 m, 0.275 m.

HALPOR—Initial value for halite porosity (dimensionless). Used in BRAGFLO. Distribution: Piecewise uniform. Range: 1.0×10^{-3} to 3×10^{-2}. Mean, median: 1.28×10^{-2}, 1.00×10^{-2}.

HALPRM—Logarithm of halite permeability (m^2). Used in BRAGFLO. Distribution: Uniform. Range: –24 to –21 (i.e., permeability range is 1×10^{-24} to 1×10^{-21} m^2). Mean, median: –22.5, –22.5. Correlation: –0.99 rank correlation with *HALCOMP* (Bulk compressibility of halite, Pa^{-1}).

WASTWICK—Increase in brine saturation of waste due to capillary forces (dimensionless). Used in BRAGFLO. Distribution: Uniform. Range: 0 to 1. Mean, median: 0.5, 0.5.

WGRCOR—Corrosion rate for steel under inundated conditions in the absence of CO_2 (m/s). Used in BRAGFLO. Distribution: Uniform. Range: 0 to 1.58×10^{-14} m/s. Mean, median: 7.94×10^{-15} m/s, 7.94×10^{-15} m/s.

WMICDFLG—Pointer variable for microbial degradation of cellulose. Used in BRAGFLO. Distribution: Discrete, with 50% 0, 25% 1, 25% 2. WMICDFLG = 0, 1, 2 implies no microbial degradation of cellulose, microbial degradation of only cellulose, microbial degradation of cellulose, plastic and rubber.

WPRTDIAM—Waste particle diameter (m). Used in CUTTINGS_S. Distribution: Loguniform. Range: 4.0×10^{-5} to 2.0×10^{-1} m. Mean, median: 2.35×10^{-2} m, 2.80×10^{-2} m.

WRBRNSAT—Residual brine saturation in waste (dimensionless). Used in BRAGFLO and BRAGFLO_DBR. Distribution: Uniform. Range: 0 to 0.552. Mean, median: 0.276, 0.276.

WTAUFAIL—Shear strength of waste (Pa). Used in CUTTINGS_S. Distribution: Uniform. Range: 0.05 to 10 Pa. Mean, median: 5.03 Pa, 5.03 Pa.

Table 4. Mechanistic Calculations Performed as Part of the 1996 WIPP PA (adapted from Table 4, Ref. 55)

BRAGFLO
Individual Calculations (6 cases; i.e., 6 different values for $\mathbf{x}_{st}$): E0 (i.e., undisturbed conditions); E1 at 350, 1000 yr (i.e., drilling intrusion through repository that penetrates pressurized brine in the Castile Fm); E2 at 350, 1000 yr (i.e., drilling intrusion through repository that does not penetrate pressurized brine in the Castile Fm); E2E1 with E2 intrusion at 800 yr and E1 intrusion at 1000 yr. *Total calculations*: 6 *nR nLHS* = 6 • 3 • 100 = 1800.
CUTTINGS_S
Individual Calculations (52 cases; i.e., 52 different values for $\mathbf{x}_{st}$): Intrusion into lower waste panel in previously unintruded (i.e., E0 conditions) repository at 100, 350, 1000, 3000, 5000, 10,000 yr; Intrusion into upper waste panel in previously unintruded repository at 100, 350, 1000, 3000, 5000, 10,000 yr; Initial E1 intrusion at 350 yr followed by a second intrusion into the same waste panel at 550, 750, 2000, 4000 or 10,000 yr; Initial E1 intrusion at 350 yr followed by a second intrusion into a different waste panel at 550, 750, 2000, 4000 or 10,000 yr; Initial E1 intrusion at 1000 yr followed by a second intrusion into the same waste panel at 1200, 1400, 3000, 5000 or 10,000 yr; Initial E1 intrusion at 1000 yr followed by a second intrusion into a different waste panel at 1200, 1400, 3000, 5000 or 10,000 yr; same 23 cases for initial E2 intrusions as for initial E1 intrusions. *Total calculations*: 52 *nR nLHS* = 52 • 3 • 100 = 15,600.
BRAGFLO_DBR
Same computational cases as for CUTTINGS_S
NUTS
Individual Calculations (15 cases; i.e., 15 different values for $\mathbf{x}_{st}$): E0; E1 at 100, 350, 1000, 3000, 5000, 7000, 9000 yr; E2 at 100, 350, 1000, 3000, 5000, 7000, 9000 yr. *Screening calculations*: 5 *nR nLHS* = 1500. *Total* NUTS *calculations*: 594. *Note*: Screening calculations were initially performed for each LHS element (i.e., E0, E1 at 350 and 1000 yr, E2 at 350 and 1000 yr, which produces the multiplier of 5 in the calculation of the number of screening calculations) to determine if the potential for a radionuclide release existed, with a full NUTS calculation only being performed when such a potential existed.
PANEL
Individual Calculations (7 cases; i.e., 7 different values for $\mathbf{x}_{st}$): E2E1 at 100, 350, 1000, 2000, 4000, 6000, 9000 yr. *Total calculations*: 7 *nR nLHS* = 7 • 3 • 100 = 2100. *Note*: Additional PANEL calculations were also performed at 100, 125, 175, 350, 1000, 3000, 5000, 7500 and 10,000 yr for Salado-dominated brines and also for Castile-dominated brines to determine dissolved radionuclide concentrations for use in the determination of direct brine releases.
SECOFL2D
Individual Calculations (2 cases; i.e., 2 different values for $\mathbf{x}_{st}$): Partially mined conditions in vicinity of repository; Fully mined conditions in vicinity of repository. *Total calculations*: 2 *nR nLHS* = 2• 3 • 100 = 600.
SECOTP2D
Individual Calculations (2 cases; i.e., 2 different values for $\mathbf{x}_{st}$): Partially mined conditions in vicinity of repository; Fully mined conditions in vicinity of repository. *Total calculations*: 2 *nR nLHS* = 2 • 3 • 100 = 600. *Note*: Each calculation is for four radionuclides: Am-241, Pu-239, Th-230, U-234. Further, calculations are done for unit releases at time 0 yr, which can then be used to construct transport results for the Culebra for arbitrary time-dependent release rates into the Culebra (Sect. 12.2, Ref. 30).