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Probability, Conditional Probability and Complementary Cumulative Distribution Functions in Performance Assessment for Radioactive Waste Disposal

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Probability, Conditional Probability and Complementary Cumulative Distribution Functions in Performance Assessment for Radioactive Waste Disposal

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ABSTRACT

A formal description of the structure of several recent performance assessments (PAs) for the Waste Isolation Pilot Plant (WIPP) is given in terms of the following three components: a probability space ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) for stochastic uncertainty, a probability space ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}) for subjective uncertainty and a function (i.e., a random variable) defined on the product space associated with ($\mathcal{S}_{st}$, $\mathcal{A}_{st}$, p_{st}) and ($\mathcal{S}_{su}$, $\mathcal{A}_{su}$, p_{su}). The explicit recognition of the existence of these three components allows a careful description of the use of probability, conditional probability and complementary cumulative distribution functions within the WIPP PA. This usage is illustrated in the context of the U.S. Environmental Protection Agency's standard for the geologic disposal of radioactive waste (40 CFR 191, Subpart B). The paradigm described in this presentation can also be used to impose a logically consistent structure on PAs for other complex systems.

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1. Introduction

The importance of an appropriate treatment of uncertainty in performance assessments (PAs) for complex systems is now widely recognized.[1-19] In particular, analyses for most complex systems such as chemical plants, nuclear power stations, radioactive waste disposal facilities and human populations involve two types of uncertainty: stochastic uncertainty and subjective uncertainty. Stochastic uncertainty arises because the system under study can behave in many different ways and is thus a property of the system. Subjective uncertainty arises from a lack of knowledge about the system and is thus a property of the analysts performing the study. Commonly used terminology for these two types of uncertainty includes aleatory, type A, irreducible and variability as alternatives to the designation stochastic and epistemic, type B, reducible and state of knowledge as alternatives to the designation subjective. Performance assessments must be carefully designed and implemented to maintain a distinction between stochastic and subjective uncertainty. Otherwise, the effects of these two types of uncertainty become commingled in a way that makes it difficult to draw useful insights from the analysis.

Probability is typically used to characterize both stochastic and subjective uncertainty (e.g., see the three analyses summarized in Ref. 20). Indeed, the use of probability is a fundamental part of PA for a complex system, with the result that PA is also referred to as probabilistic risk assessment (PRA). Yet, when the documentation of most PAs is examined, little is typically found that is suggestive of the conceptual material covered in a textbook on probability. This is unfortunate because having a clear conceptual model for the probabilistic basis of an analysis helps in understanding the design and implementation of the analysis, in avoiding conceptual errors, and in relating analysis procedures to similar procedures used in other contexts.

The purpose of this presentation is to provide a formal probabilistic description of a PA involving stochastic and subjective uncertainty. This description will be given in the context of several recent PAs for the Waste Isolation Pilot Plant (WIPP).[21-29] However, the underlying concepts and associated structure are relevant to PAs for any system that involves both stochastic and subjective uncertainty.

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2. Probability

Probability is more than a number between 0 and 1. Rather, there are three elements in the development of probability: (1) a set $\mathcal{S}$ that contains everything that could occur for the particular "universe" under construction, (2) a suitably restricted set $\mathscr{S}$ of subsets of $\mathcal{S}$, called a Borel or σ-algebra, and (3) a function p defined for elements of $\mathscr{S}$ that actually defines probability.[30-31] In particular, $\mathscr{S}$ has the properties that (1) if $\mathcal{E} \in \mathscr{S}$, then $\mathcal{E}^c \in \mathscr{S}$, where the superscript c is used to denote the complement of $\mathcal{E}$, and (2) if $\{\mathcal{E}_i\}$ is a countable collection of elements of $\mathscr{S}$, then $\cup_i \mathcal{E}_i$ and $\cap_i \mathcal{E}_i$ are also elements of $\mathscr{S}$, and p has the properties that (1) $p(\mathcal{S}) = 1$, (2) if $\mathcal{E} \in \mathscr{S}$, then $0 \le p(\mathcal{E}) \le 1$, and (3) if $\mathcal{E}_1, \mathcal{E}_2, \ldots$ is a sequence of disjoint sets from $\mathscr{S}$ (i.e., $\mathcal{E}_i \cap \mathcal{E}_j = \phi$ if $i \neq j$), then $p(\cup_i \mathcal{E}_i) = \Sigma_i\, p(\mathcal{E}_i)$. The triple $(\mathcal{S}, \mathscr{S}, p)$ is called a probability space. In the terminology of probability theory, $\mathcal{S}$ is the sample space, the elements of $\mathcal{S}$ are elementary events, and the subsets of $\mathcal{S}$ contained in $\mathscr{S}$ are events. In most applied problems, the function p defined on $\mathscr{S}$ is replaced by a density function d such that, if $\mathcal{E} \in \mathscr{S}$, then

$$p(\mathcal{E}) = \int_{\mathcal{E}} d(\mathbf{x})\, dV. \tag{1}$$

In a careful development of probability, the preceding integral would be a Lebesgue integral, but for our purposes it can be assumed to be the Riemann integral of elementary calculus. The properties of the set $\mathscr{S}$ enter into the formal development of the concept of integration over $\mathcal{S}$. The notation dV is used in Eq. (1) because $\mathcal{S}$ is multidimensional (e.g., $\mathcal{S} \subset R^n$) in most problems of interest.

Problems involving probability usually relate to the behavior of a function f defined on the sample space $\mathcal{S}$ associated with a probability space $(\mathcal{S}, \mathscr{S}, p)$. For example, the expected value of f is given by

$$E(f) = \int_{\mathcal{S}} f(\mathbf{x}) d(\mathbf{x}) dV. \tag{2}$$

Similarly, the complementary cumulative distribution function (CCDF) associated with f is given by

$$CCDF(R) = \int_{\mathcal{S}} \delta_R[f(\mathbf{x})] d(\mathbf{x}) dV, \tag{3}$$

where

$$\delta_R[z] = \begin{cases} 1 & \text{if } z > R \\ 0 & \text{if } z \le R \end{cases} \tag{4}$$

and $CCDF(R)$ is the probability that a value of R will be exceeded by f. In an unfortunate but widely-used terminology, f is referred to as a random variable.

The CCDF defined in Eq. (3) is defined over the entire sample space $\mathcal{S}$. It is also possible to define CCDFs conditional on the occurrence of subsets of $\mathcal{S}$. In particular, the CCDF associated with f conditional on the occurrence of a subset $\mathcal{E}$ of $\mathcal{S}$ is given by

$$CCDF(R|\mathcal{E}) = \int_{\mathcal{E}} \delta_R[f(\mathbf{x})]d(\mathbf{x})dV \Big/ \int_{\mathcal{E}} d(\mathbf{x})dV, \tag{5}$$

where δ_R is defined in Eq. (4) and $CCDF(R|\mathcal{E})$ is the probability that a value of R will be exceeded by f given that consideration is restricted to the set $\mathcal{E}$. The probabilities $CCDF(R|\mathcal{E})$ are conditional probabilities because of the restriction of consideration to the subset $\mathcal{E}$ of $\mathcal{S}$.

An additional important concept that arises in PAs for complex systems is that of a product space. Many problems involve more than one probability space. For example, two probability spaces $(\mathcal{S}_1, \mathcal{A}_1, p_1)$ and $(\mathcal{S}_2, \mathcal{A}_2, p_2)$ might be involved in the formulation of a problem. Then, a third probability space $(\mathcal{S}, \mathcal{A}, p)$ can be obtained by combining $(\mathcal{S}_1, \mathcal{A}_1, p_1)$ and $(\mathcal{S}_2, \mathcal{A}_2, p_2)$, where

$$\mathcal{S} = \mathcal{S}_1 \times \mathcal{S}_2 = \{[\mathbf{x}_1, \mathbf{x}_2] : \mathbf{x}_1 \in \mathcal{S}_1, \mathbf{x}_2 \in \mathcal{S}_2\}, \tag{6}$$

$$\mathcal{A} = \mathcal{A}_1 \times \mathcal{A}_2 = \{\mathcal{E} : \mathcal{E} = \mathcal{E}_1 \times \mathcal{E}_2, \text{ where } \mathcal{E}_1 \in \mathcal{A}_1, \mathcal{E}_2 \in \mathcal{A}_2\}, \tag{7}$$

$$p(\mathcal{E}) = p_1(\mathcal{E}_1)p_2(\mathcal{E}_2) \quad \text{for } \mathcal{E} = \mathcal{E}_1 \times \mathcal{E}_2 . \tag{8}$$

The definition of $p(\mathcal{E})$ in Eq. (8) implies that $(\mathcal{S}_1, \mathcal{A}_1, p_1)$ and $(\mathcal{S}_2, \mathcal{A}_2, p_2)$ are independent in the sense that the occurrence of elements of $\mathcal{S}_1$ has no effect on the occurrence of elements of $\mathcal{S}_2$ and vice versa. If such is not the case, then more involved relationships are required to define p.

3. Probability in PAs for the WIPP

Now that a few basic ideas from probability have been introduced, the use of probability in PAs for complex systems is considered. This usage will be motivated and illustrated by procedures used in several recent PAs for the WIPP (i.e., in 1991[21-24] and 1992[25-29]). The use of probability in these PAs derives from the EPA Containment Requirement 40 CFR 191.13,[33,34] which follows:

§ 191.13 Containment Requirements.

(a) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based upon performance assessments, that cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall:

(1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A); and

(2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix A).

(b) Performance assessments need not provide complete assurance that the requirements of 191.13(a) will be met. Because of the long time period involved and the nature of the events and processes of interest, there will inevitably be substantial uncertainties in projecting disposal system performance. Proof of the future performance of a disposal system is not to be had in the ordinary sense of the word in situations that deal with much shorter time frames. Instead, what is required is a reasonable expectation, on the basis of the record before the implementing agency, that compliance with 191.13(a) will be achieved.

Containment Requirement 191.13(a) requires that the CCDF for normalized release to the accessible environment fall below a boundary line[35-38] defined by the points (0.1,1) and (0.001,10) as indicated in Fig 1. Construction of this CCDF requires a probability space. In the WIPP PA, this probability space is assumed to derive from various disruptive events that conceivably could occur at the WIPP over the next 10,000 yr. The defining character of these events is that their occurrence involves a relatively rapid change in conditions at the WIPP (e.g., volcanism, meteor impact, drilling intrusions, ...). In the WIPP PA, as in many other analyses, the uncertainty indtroduced by the possible occurrence of such disruptions is referred to as stochastic uncertainty and is characterized by a probability space $(\mathcal{S}_{st}, \mathcal{I}_{st}, p_{st})$.

Review work has indicated that drilling intrusions are the only disruptions at the WIPP with sufficient probability to be relevant to assessing compliance with 191.13(a) (Ref. 21, Chapt. 4). Therefore, the probability space $(\mathcal{S}_{st}, \mathcal{I}_{st}, p_{st})$ for stochastic uncertainty is used to characterize the occurrence of drilling intrusions. In the computational implementation of recent PAs for the WIPP, the elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$ have been vectors of the form

$$\mathbf{x}_{st} = [t_1, x_1, l_1, t_2, x_2, l_2, \ldots, t_n, x_n, l_n, 0, 0, 0, \ldots], \tag{9}$$

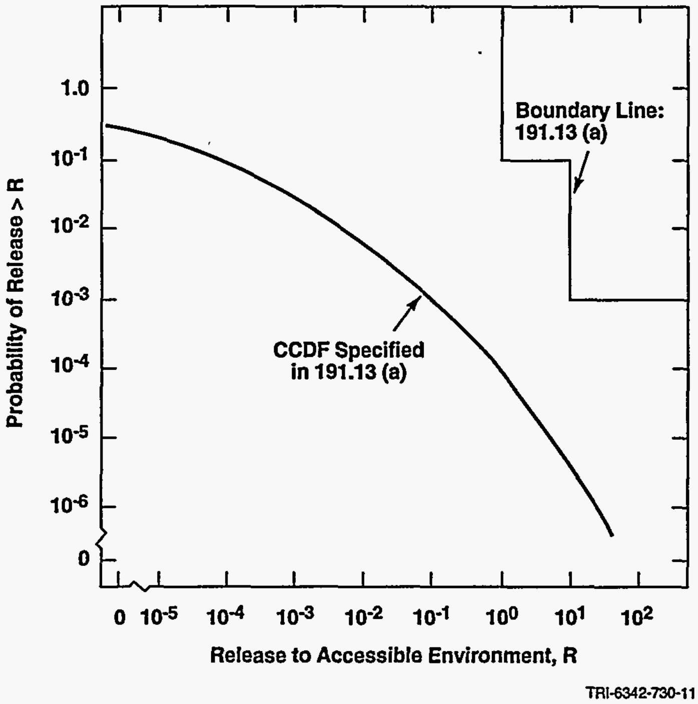

Fig. 1. Comparison of CCDF for normalized release to the accessible environment with boundary line specified in 191.13(a).

where t_i is the time of the i^{th} drilling intrusion, x_i is the location of the i^{th} drilling intrusion, l_i is the activity level of waste penetrated by the i^{th} drilling intrusion, and n is the number of drilling intrusions. The function p_{st} is defined in terms of the rate constant λ in a Poisson model for drilling intrusions, the area of pressurized brine beneath the waste panels, and the repository area occupied by waste of each activity level.[39,40] Given the definition of $\mathbf{x}_{st}$ in Eq. (9), $\mathcal{S}_{st}$ is a subset of R^{∞}. However, because of upper bounds placed on λ, n has been assumed to satisfy the bound $n \leq nBH$ in recent PAs for the WIPP, in which case $\mathcal{S}_{st}$ is a subset of R^{3nBH} and, as an example, a subset of R^{30} if $nBH = 10$.

The CCDF specified in 191.13(a) is obtained by integrating over $\mathcal{S}_{st}$ as indicated in Eq. (3). Specifically, the CCDF for comparison with the EPA release limits is given by

$$CCDF(R) = \int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st})\right] d_{st}(\mathbf{x}_{st})\, dV_{st} \tag{10}$$

$$\doteq \sum_{i=1}^{nS} \delta_R\left[f(\mathbf{x}_{st,i})\right] p_{st}(\mathcal{S}_{st,i}), \tag{11}$$

where R corresponds to normalized release to the accessible environment, the function f corresponds to the combined operation of models of the form indicated in Fig. 2 to predict the normalized release associated with an element $\mathbf{x}_{st}$

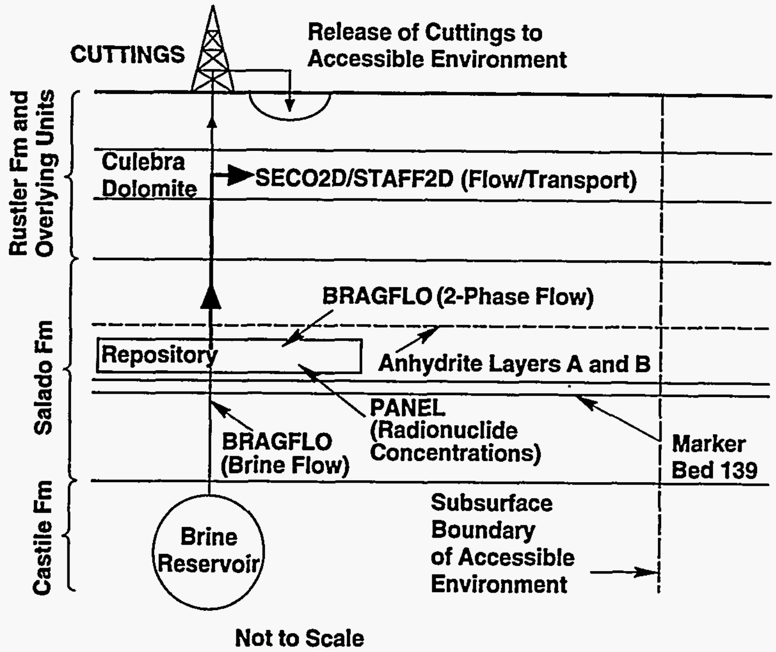

Fig. 2. Computer programs used in 1991 WIPP PA. Additional information on the individual programs is available as indicated: BRAGFLO (Ref. 22, Chapt. 5; Ref. 41, Sect. 3.1), CUTTINGS (Ref. 22, Chapt. 7; Ref. 41, Sect. 3.5; Ref. 42), PANEL (Ref. 22, Chapt. 5; Ref. 41, Sect. 3.2), SECO2D (Ref. 22, Chapt. 6; Ref. 41, Sect. 3.3; Ref. 43), STAFF2D (Ref. 22, Chapt. 6; Ref. 41, Sect. 3.4; Ref. 44).

of $\mathcal{S}_{st}$, $\cup_i \mathcal{S}_{st,i} = \mathcal{S}_{st}$, $\mathcal{S}_{st,i} \cap \mathcal{S}_{st,j} = \phi$ if $i \neq j$, and $\mathbf{x}_{st,i} \in \mathcal{S}_{st,i}$. The approximation to the integral in Eq. (1) indicated in Eq. (11) is calculated by the program CCDFPERM[40] in recent PAs for the WIPP.

Once $(\mathcal{S}_{st}, \mathcal{s}_{st}, p_{st})$ and f have been developed, the first of several types of conditional CCDFs is possible. In particular, a CCDF conditional on the occurrence of a specific subset $\mathcal{E}$ of $\mathcal{S}_{st}$ can be determined. For example, let $\mathcal{E}_1$ be defined by

$$\mathcal{E}_1 = \{\mathbf{x}_{st}: \mathbf{x}_{st} \in \mathcal{S}_{st} \text{ and involves one or more drilling intrusions}\}, \tag{12}$$

which is equivalent to defining $\mathcal{E}_1$ to be the set of all vectors of the form defined in Eq. (9) with $n \geq 1$. The corresponding conditional CCDF is given by

$$CCDF(R \mid \mathcal{E}_1) = \int_{\mathcal{E}_1} \delta_R\left[f(\mathbf{x}_{st})\right] d_{st}(\mathbf{x}_{st}) dV_{st} \Big/ \int_{\mathcal{E}_1} d_{st}(\mathbf{x}_{st}) dV_{st}, \tag{13}$$

where $CCDF(R \mid \mathcal{E}_1)$ is the conditional probability of exceeding a normalized release of size R given that at least one drilling intrusion has occurred. Examples of CCDFs conditional on the set $\mathcal{E}_1$ in Eq. (12) are shown in Fig. 3.

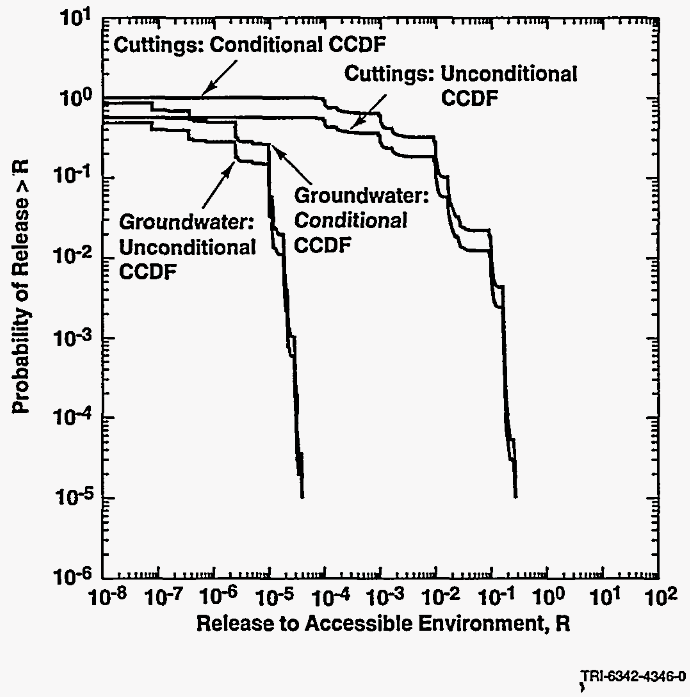

Fig. 3. Original (unconditional) CCDFs and CCDFs conditional on one or more drilling intrusions (i.e., on the set $\mathcal{E}_1$ in Eq. (12)) for release to the accessible environment due to groundwater transport and release to the accessible environment due to cuttings removal for sample element 46 in 1991 WIPP PA.

If there was no uncertainty as to how the function f and density d_{st} in Eq. (10) should be defined, then the CCDF required in 191.13(a) could be calculated and compared with the specified boundary line. With complete certainty, 191.13(a) would either be met or not met, and there would be no additional uncertainty to be considered in the analysis. However, this type of certainty never exists in an analysis for a complex system, which is where 191.13(b) enters the analysis and leads to an additional probability space.

Containment Requirement 191.13(b) requires a "reasonable expectation" that compliance with 191.13(a) will be achieved. The goal in recent PAs for the WIPP has been to assess this reasonable expectation on the basis of the effects that fixed, but poorly known, quantities have on the location of the CCDF specified in 191.13(a). To this end, the function f and density d_{st} in Eq. (10) were developed so that $f(\mathbf{x}_{st})$ and $d_{st}(\mathbf{x}_{st})$ depend on quantities that are believed to have fixed values (at least within the resolution of the modeling being used). In other words, f and d_{st} are treated as being of the form $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ and $d_{st}(\mathbf{x}_{st}|\mathbf{x}_{su})$, where $\mathbf{x}_{st} \in \mathcal{S}_{st}$ and $\mathbf{x}_{su}$ is a vector of fixed, but poorly known, quantities. Distributions are then assigned to the elements of $\mathbf{x}_{su}$ to characterize where their true, but unknown, values are believed to be located. In turn, the location of the distribution of CCDFs that results from the uncertainty in $\mathbf{x}_{su}$ provides a measure of the assurance with which 191.13(a) can be met. The development of distributions for the elements of $\mathbf{x}_{su}$ is still in progress in the WIPP PA,[23,27] with the result that the PA has not yet arrived at the point where all distributions in use can be viewed a providing representations for where "true, but unknown, values are believed to be located." In particular, the analysis is still at a stage where some distributions are assigned primarily to help assess the sensitivity of analysis outcomes to the associated input variable.

Definition of distributions for the elements of $\mathbf{x}_{su}$ defines the probability space $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$ for subjective uncertainty. Here, subjective uncertainty is used to designate a lack of knowledge about a fixed, but unknown, quantity. The study of subjective uncertainty is the primary domain of classical statistics, although many analyses for complex systems find that they must rely heavily on expert-review processes[45-48] to assess subjective uncertainty [i.e., to define $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$]. In the 1991 WIPP PA, $\mathbf{x}_{su}$ contained the 45 variables indicated in Table 1; thus, $\mathcal{S}_{su}$ is a subset of R^{45}. For notational ease, integrals over elements of $\mathscr{S}_{su}$ will be expressed with the density function d_{su}. Thus,

$$p(\mathcal{E}) = \int_{\mathcal{E}} d_{su}(\mathbf{x}_{su}) dV_{su} \tag{14}$$

for $\mathcal{E} \in \mathscr{S}_{su}$.

Table 1. Examples of Imprecisely Known Variables Considered in 1991 WIPP PA (adapted from Table 3-1 of Ref. 24, App. A of Ref. 41 and Table VIII of Ref. 49, which list all 45 variables considered in the 1991 WIPP PA). The variables indicated in this table and their associated distributions define the probability space $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$ for subjective uncertainty.

	Variable	Definition
1	*BHPERM*	Borehole permeability. Range: 1×10^{-14} to 1×10^{-11} m^2. Distribution: Lognormal.
2	*BPPRES*	Initial pressure of pressurized brine pocket in Castile Formation: Range: 1.1×10^7 to 2.1×10^7 Pa. Distribution: Piecewise linear.
3	*BPSTOR*	Bulk storativity of pressurized brine pocket in Castile Formation: Range: 2×10^{-2} to 2 m^3. Distribution: Lognormal.
4	*BPAREAFR*	Fraction of waste panel area underlain by a pressurized brine pocket (dimensionless). Range: 2.5×10^{-1} to 5.52×10^{-1}. Distribution: Approximately uniform.
		⋮
23	*LAMBDA*	Rate constant in Poisson model for drilling intrusions. Range: 0 to 1.04×10^{-11} s^{-1}. Distribution: Uniform.
		⋮
45	*VWOOD*	Fraction of total waste volume that is occupied by IDB (Integrated Data Base)[50] combustible waste category (dimensionless). Range: 2.84×10^{-1} to 4.84×10^{-1}. Distribution: Normal.

At this point, the WIPP PA involves two probability spaces, $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ and $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$, and the actual object of study becomes the product space $(\mathcal{S}, \mathcal{J}, p)$ derived from these two individual spaces [see Eqs. (6) - (8)]. Definition of the probability function p associated with this product space is actually more complicated than indicated in Eq. (8) because elements of $\mathcal{S}_{su}$ affect the definition of p_{st}. In particular, p has the form

$$p(\mathcal{E}) = \int_{\mathcal{E}} d(\mathbf{x})dV, \quad \mathbf{x} = [\mathbf{x}_{st}, \mathbf{x}_{su}]$$

$$= \int_{\mathcal{E}_{su}} \left[\int_{\mathcal{E}_{st}} d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su}) dV_{st} \right] d_{su}(\mathbf{x}_{su}) dV_{su}, \tag{15}$$

where $\mathcal{E} = \mathcal{E}_{st} \times \mathcal{E}_{su} \in \mathcal{J}$, d is the density function associated with p, and d_{st} is now a function of both $\mathbf{x}_{st}$ and $\mathbf{x}_{su}$ (Table 2).

Three different CCDFs associated with the product space containing $\mathcal{S}_{st} \times \mathcal{S}_{su}$ for normalized release to the accessible environment are presented in PAs for the WIPP: an unconditional CCDF based on the entire product space, a CCDF conditional on the occurrence of a specific element of $\mathcal{S}_{su}$, and a CCDF conditional on the occurrence of a specific element of $\mathcal{S}_{st}$. In addition, a cumulative distribution function (CDF) based on the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ also plays an important role. Each of these cases is now discussed.

Table 2. Definition of Density Functions for $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$, $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ and $(\mathcal{S}, \mathcal{J}, p)$.

Density Functions Assumed to be Known		
$d_{su}(\mathbf{x}_{su})$	=	density function for $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$
$d_{st}(\mathbf{x}_{st} \vert \mathbf{x}_{su})$	=	density function for $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ given $\mathbf{x}_{su}$
Constructed Density Functions		
$d(\mathbf{x}_{st}, \mathbf{x}_{su})$	=	density function for $(\mathcal{S}, \mathcal{J}, p)$
	=	$d_{st}(\mathbf{x}_{st} \vert \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})$
$d_{st}(\mathbf{x}_{st})$	=	density function for $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$
	=	$\int_{\mathcal{S}_{su}} d(\mathbf{x}_{st}, \mathbf{x}_{su}) dV_{su}$
	=	$\int_{\mathcal{S}_{su}} d_{st}(\mathbf{x}_{st} \vert \mathbf{x}_{su}) d_{su}(\mathbf{x}_{su}) dV_{su}$
$d_{su}(\mathbf{x}_{su} \vert \mathbf{x}_{st})$	=	density function for $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ given $\mathbf{x}_{st}$
	=	$d(\mathbf{x}_{st}, \mathbf{x}_{su}) / d_{st}(\mathbf{x}_{st}),\ d_{st}(\mathbf{x}_{st}) \neq 0$
	=	$d_{st}(\mathbf{x}_{st} \vert \mathbf{x}_{su}) d_{su}(\mathbf{x}_{su}) / \int_{\mathcal{S}_{su}} d_{st}(\mathbf{x}_{st} \vert \mathbf{x}_{su}) d_{du}(\mathbf{x}_{su}) dV_{su}$

3.1 Unconditional CCDF on Product Space for $\mathcal{S}_{st} \times \mathcal{S}_{su}$

The unconditional CCDF based on the entire product space is given by

$$
\begin{aligned}
CCDF(R) &= \int_{\mathcal{S}} \delta_R[f(\mathbf{x})]\, d(\mathbf{x})\, dV, \quad \mathcal{S} = \mathcal{S}_{st} \times \mathcal{S}_{su}, \ \mathbf{x} = [\mathbf{x}_{st}, \mathbf{x}_{su}] \\
&= \int_{\mathcal{S}_{su}} \left[\int_{\mathcal{S}_{st}} \delta_R[f(\mathbf{x}_{st}, \mathbf{x}_{su})]\, d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su})\, dV_{st} \right] d_{su}(\mathbf{x}_{su})\, dV_{su},
\end{aligned} \tag{16}
$$

where $CCDF(R)$ is the probability that a normalized release of size R will be exceeded. In the 1991 WIPP PA, the function f derives from the combined operation of the CUTTINGS, BRAGFLO, PANEL, SECO2D and STAFF2D models as indicated in Fig. 2; in the 1992 WIPP PA, the STAFF2D model was replaced by the SECOTP model (Ref. 26, App. C; Ref. 28, Chapt. 6). The CCDF in Eq. (16) is designated as the mean CCDF in PAs for the WIPP (see Figs. 4 and 5, with an approximation to the CCDF defined in Eq. (16) appearing in Fig. 5). The reason for the designation "mean CCDF" will be discussed later.

The integral in Eq. (16) is too complicated to be evaluated with a closed-form procedure. Rather, a numerical approximation must be used. In the WIPP PA, a two stage procedure is used to approximate this integral. In the first stage, Monte Carlo techniques are used to approximate the outer integral in Eq. (16). Specifically, a Latin hypercube sample[51]

$$
\mathbf{x}_{su,k}, \ k = 1, 2, \ldots, nLHS, \tag{17}
$$

is generated from the sample space $\mathcal{S}_{su}$ associated with the probability space $(\mathcal{S}_{su}, \mathcal{L}_{su}, p_{su})$, which leads to the following approximation to $CCDF(R)$:

$$
CCDF(R) \doteq \sum_{k=1}^{nLHS} \int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su,k})\right] d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su,k})\, dV_{st} \,/\, nLHS. \tag{18}
$$

In the WIPP PA, the Latin hypercube sample is generated with the LHS program[52] and the mechanics of performing the indicated summation take place in the CCDFPERM program.[40] In the second stage of the procedure, the integrals in Eq. (18) are evaluated with an importance sampling procedure (Ref. 53, Sect. 5.4) that involves the subdivision of the sample space $\mathcal{S}_{st}$ associated with the probability space $(\mathcal{S}_{st}, \mathcal{L}_{st}, p_{st})$ into a sequence $\mathcal{S}_{st,i}$, $i = 1, 2, \ldots, nS$, of disjoint subsets such that $\cup_i \mathcal{S}_{st,i} = \mathcal{S}_{st}$. Although the notation in use does not explicitly indicate it, $(\mathcal{S}_{st}, \mathcal{L}_{st}, p_{st})$ actually changes from sample element to sample element (i.e., is a function of $\mathbf{x}_{su}$) due to the dependence of p_{st} on variables contained in $\mathbf{x}_{su}$, with the result that the sets $\mathcal{S}_{st,i}$ and the probabilities $p_{st}(\mathcal{S}_{st,i})$ can also change from sample element to sample element. Once the $\mathcal{S}_{st,i}$ are defined, the approximation to $CCDF(R)$ becomes

$$
CCDF(R) \doteq \sum_{k=1}^{nLHS} \left[\sum_{i=1}^{nS} \delta_R\left[f(\mathbf{x}_{st,i}, \mathbf{x}_{su,k})\right] p_{st}(\mathcal{S}_{st,i}) \right] / \, nLHS, \tag{19}
$$

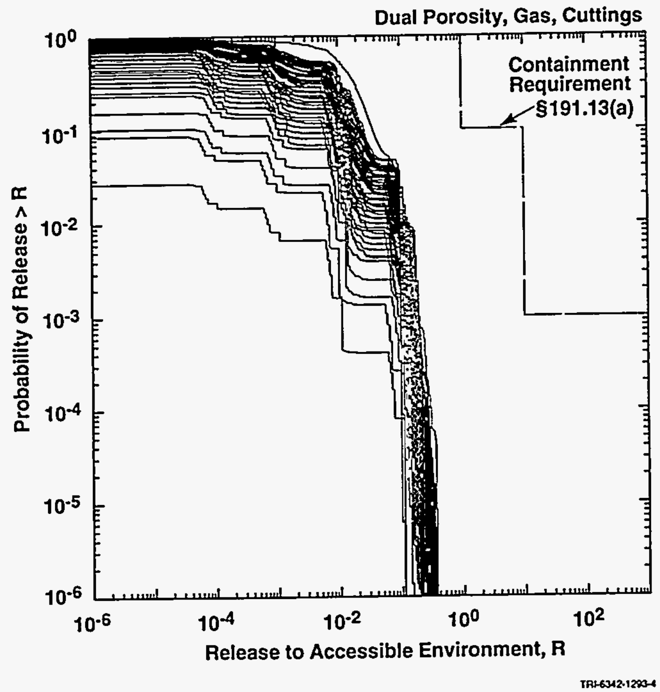

Fig. 4. Distribution of CCDFs for normalized release to the accessible environment including both cuttings removal and groundwater transport with gas generation in the repository and a dual-porosity transport model in the Culebra Dolomite (Ref. 24, Fig. 2.2-2; Ref. 49, Fig. 2).

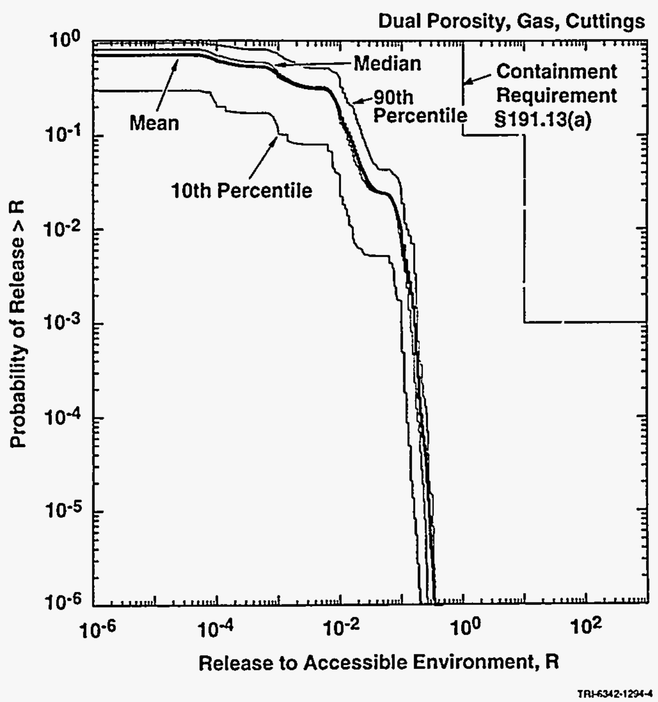

Fig. 5. Mean and percentile curves for distribution of CCDFs shown in Fig. 4 (Ref. 24, Fig. 4.1-1; Ref. 49, Fig. 6).

where $\mathbf{x}_{st,i} \in \mathcal{S}_{st,i}$ and $p_{st}(\mathcal{S}_{st,i})$ is defined by

$$p_{st}\left(\mathcal{S}_{st,i}\right) = \int_{\mathcal{S}_{st,i}} d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su,k})\, dV_{st}. \tag{20}$$

In terms of implementation, $f(\mathbf{x}_{st}, \mathbf{x}_{su,k})$ is calculated with CUTTINGS, BRAGFLO, PANEL, SECO2D and STAFF2D for a relatively small number of elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$; the results for these elements are then used to construct (i.e., estimate) $f(\mathbf{x}_{st,i}, \mathbf{x}_{su,k})$ for the large number of $\mathbf{x}_{st,i}$ involved in the summation in Eq. (19).[40] This construction process takes place in the program CCDFPERM, as does the evaluation of the probability $p_{st}(\mathcal{S}_{st,i})$ in Eq. (20). The mean CCDF in Fig. 5 was produced by the calculation shown in Eq. (19).

3.2 CCDF Conditional on Element of $\mathcal{S}_{su}$

The construction of a CCDF conditional on the occurrence of a specific element of $\mathcal{S}_{su}$ is now considered. It is useful to begin by considering the more general case of a CCDF conditional on the occurrence of an arbitrary subset $\mathcal{E}_{su}$ of $\mathcal{S}_{su}$. The corresponding conditional CCDF for normalized release to the accessible environment has the form shown in Eq. (5), where the probability space under consideration is the product space associated with $\mathcal{S}_{st} \times \mathcal{S}_{su}$. As a result, the CCDF is actually conditional on the occurrence of $\mathcal{S}_{st} \times \mathcal{E}_{su}$. Specifically,

$$\begin{aligned} CCDF\left(R | \mathcal{S}_{st} \times \mathcal{E}_{su}\right) &= \int_{\mathcal{S}_{st} \times \mathcal{E}_{su}} \delta_R[f(\mathbf{x})]\, d(\mathbf{x}) dV \Big/ \int_{\mathcal{S}_{st} \times \mathcal{E}_{su}} d(\mathbf{x}) dV, \;\; \mathbf{x} = [\mathbf{x}_{st}, \mathbf{x}_{su}] \\ &= \int_{\mathcal{E}_{su}} \int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su})\right] d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})\, dV_{st}\, dV_{su} \\ &\quad \Big/ \int_{\mathcal{E}_{su}} \int_{\mathcal{S}_{st}} d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})\, dV_{st}\, dV_{su}, \end{aligned} \tag{21}$$

where $CCDF\left(R | \mathcal{S}_{st} \times \mathcal{E}_{su}\right)$ is the probability that a normalized release of size R will be exceeded conditional on the occurrence of $\mathcal{S}_{st} \times \mathcal{E}_{su}$.

For a CCDF conditional on the occurrence of a specific element $\tilde{\mathbf{x}}_{su}$ of $\mathcal{S}_{su}$, the set $\mathcal{E}_{su}$ will contain only $\tilde{\mathbf{x}}_{su}$, with the outcome that the integrals in the numerator and denominator of Eq. (21) will be zero. As a result, Eq. (21) cannot be applied directly to obtain $CCDF\left(R | \mathcal{S}_{st} \times \{\tilde{\mathbf{x}}_{su}\}\right)$ Instead, the desired probability is obtained by taking the limit of the expression in Eq. (21) as the size of the set $\mathcal{E}_{su}$ containing $\tilde{\mathbf{x}}_{su}$ approaches a volume of zero (i.e., as $V(\mathcal{E}_{su}) \rightarrow 0$). Specifically, $CCDF\left(R | \mathcal{S}_{st} \times \{\tilde{\mathbf{x}}_{su}\}\right)$ is defined by the limit

$$CCDF\left(R \mid \mathcal{S}_{st} \times \{\tilde{\mathbf{x}}_{st}\}\right) = \underset{V(\mathcal{E}_{su}) \to 0}{\text{limit}} \left\{ \int_{\mathcal{E}_{su}} \int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su})\right] d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})\, dV_{st}\, dV_{su} \right.$$

$$\left. / \int_{\mathcal{E}_{su}} \int_{\mathcal{S}_{st}} d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})\, dV_{st}\, dV_{su} \right\}$$

$$= \underset{V(\mathcal{E}_{su}) \to 0}{\text{limit}} \left\{ \left[\int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \overline{\mathbf{x}}_{su})\right] d_{st}(\mathbf{x}_{st} \mid \overline{\mathbf{x}}_{su})\, dV_{st} \right] d_{su}(\overline{\mathbf{x}}_{su})\, V(\mathcal{E}_{su}) \right.$$

$$\left. / \left[\int_{\mathcal{S}_{st}} d_{st}(\mathbf{x}_{st} \mid \hat{\mathbf{x}}_{su})\, dV_{st} \right] d_{su}(\hat{\mathbf{x}}_{su})\, V(\mathcal{E}_{su}) \right\}$$

$$\left[\text{by mean value theorem with } \overline{\mathbf{x}}_{su}, \hat{\mathbf{x}}_{su} \in \mathcal{E}_{su}\right]$$

$$= \underset{V(\mathcal{E}_{su}) \to 0}{\text{limit}} \left[\int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \overline{\mathbf{x}}_{su})\right] d_{st}(\mathbf{x}_{st} \mid \overline{\mathbf{x}}_{su})\, dV_{st} \right] \left[d_{su}(\overline{\mathbf{x}}_{su}) / d_{su}(\hat{\mathbf{x}}_{su}) \right]$$

$$= \int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \tilde{\mathbf{x}}_{su})\right] d_{st}(\mathbf{x}_{st} \mid \tilde{\mathbf{x}}_{su})\, dV_{st}, \tag{22}$$

provided the functions involved are "reasonably" behaved.

The expression $CCDF\left(R \mid \mathcal{S}_{st} \times \{\tilde{\mathbf{x}}_{su}\}\right)$ as defined by the integral in Eq. (22) gives the probability of exceeding a normalized release of size R conditional on the occurrence of the element $\tilde{\mathbf{x}}_{su}$ of $\mathcal{S}_{su}$. In PAs for the WIPP, this probability is approximated by

$$CCDF\left(R \mid \mathcal{S}_{st} \times \{\tilde{\mathbf{x}}_{su}\}\right) \doteq \sum_{i=1}^{nS} \delta_R\left[f(\mathbf{x}_{st,i}, \tilde{\mathbf{x}}_{su})\right] p_{st}(\mathcal{S}_{st,i}) \tag{23}$$

with use of the same notation as in Eq. (19). In particular, the probability of exceeding a normalized release of size R conditional on the occurrence of a sample element $\mathbf{x}_{su,k}$ of the form indicated in Eq. (17) is

$$CCDF\left(R \mid \mathcal{S}_{st} \times \{\mathbf{x}_{su,k}\}\right) \doteq \sum_{i=1}^{nS} \delta_R\left[f(\mathbf{x}_{st,i}, \mathbf{x}_{su,k})\right] p_{st}(\mathcal{S}_{st,i}). \tag{24}$$

Plots of the resultant CCDFs for the individual sample elements in the 1991 WIPP PA appear in Fig. 4. The calculation indicated in Eq. (24) to obtain the CCDFs in Fig. 4 is performed in the program CCDFPERM.[40]

The CCDF discussed in Sect. 3.1 is often referred to as a "mean CCDF" because it can be viewed as the mean of the CCDFs discussed in this section. In particular, the integral for $CCDF\left(R \mid \mathcal{S}_{st} \times \{\tilde{\mathbf{x}}_{su}\}\right)$ in Eq. (22) is the inner integral in Eq. (16).

3.3 CDF Based on $\mathcal{S}_{su}$

The expression $CCDF(R \mid \mathcal{S}_{st} \times \{\mathbf{x}_{su}\})$ is a function defined on $\mathcal{S}_{su}$ for each value of R. Thus, this expression has a distribution that derives from the probability space ($\mathcal{S}_{su}$, $\mathcal{S}_{su}$, p_{su}). For notational reasons, this distribution is best expressed as a cumulative distribution function (CDF). In particular, the probability that $CCDF(R \mid \mathcal{S}_{st} \times \{\mathbf{x}_{su}\})$ is less than or equal to p is given by

$$\begin{aligned} CDF(p,R) &= 1 - \int_{\mathcal{S}_{su}} \delta_p\left[CCDF\left(R \mid \mathcal{S}_{st} \times \{\mathbf{x}_{su}\}\right)\right] d(\mathbf{x}_{su})\, dV_{su} \\ &= 1 - \int_{\mathcal{S}_{su}} \delta_p\left\{\int_{\mathcal{S}_{st}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su})\right] d_{st}\left(\mathbf{x}_{st} \mid \mathbf{x}_{su}\right) dV_{st}\right\} d(\mathbf{x}_{su})\, dV_{su}, \end{aligned} \tag{25}$$

where δ_p is defined as indicated in Eq. (4). The CDFs defined by Eq. (25) are characterizing the uncertainty in the exceedance probabilities that are used in comparisons with the boundary line specified in 191.13(a). The probability space ($\mathcal{S}_{su}$, $\mathcal{S}_{su}$, p_{su}) characterizes how well we (i.e., all the analysts involved) know the appropriate values for use in the modeling system employed in a PA for the WIPP. The uncertainty in this input translates into corresponding uncertainty in quantities predicted by the PA. Among these uncertain quantities are the exceedance probabilities associated with normalized releases of different sizes. The CDFs defined by Eq. (25) characterize a degree of belief with respect to where these exceedance probabilities are located and thus provide a measure of the assurance requested in 191.13(b) that 191.13(a) will be met.

As is the case for all integrals over probability spaces in PAs for the WIPP, the integral in Eq. (25) must be approximated numerically. Specifically, the following approximation is used:

$$CDF(p,R) \doteq 1 - \sum_{k=1}^{nLHS} \delta_p\left\{\sum_{i=1}^{nS} \delta_R\left[f\left(\mathbf{x}_{st,i}, \mathbf{x}_{su,k}\right)\right] p_{st}\left(\mathcal{S}_{st,i}\right)\right\} / nLHS, \tag{26}$$

where notation is the same as used in Eq. (19). Further, Eq. (19) provides an approximation to the expected (i.e., mean) value of $CCDF(R \mid \mathcal{S}_{st} \times \{\mathbf{x}_{su}\})$, where this expectation derives from ($\mathcal{S}_{su}$, $\mathcal{S}_{su}$, p_{su}). As an example, the CDFs that result for the results summarized in Fig. 4 and values of R = 0.001, 0.01 and 0.1 are shown in Fig. 6. The preceding procedure for estimating the integral in Eq. (25) for a given value of R is equivalent to determining the number $nE(\leq p)$ of CCDFs that have an exceedance probability less than or equal to p and then defining $CDF(p,R)$ to be $nE(\leq p)/nLHS$. The percentile curves (i.e., 10th, 50th (median), 90th) and mean curve in Fig. 5 result from connecting the corresponding percentile and mean values for individual normalized releases. Thus, these curves provide a compact summary for distributions of the form shown in Fig. 6. A CDF is used to represent the uncertainty in exceedance probabilities so that the distributions in Fig. 6 will have the same orientation as the percentile curves in Fig. 5.

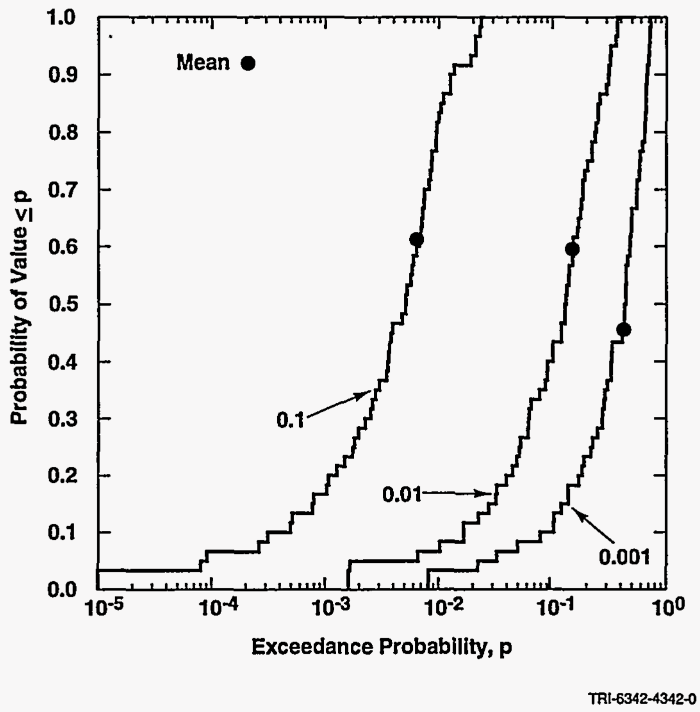

Fig. 6. Estimated CDFs for exceedance probabilities associated with normalized releases to the accessible environment of $R = 0.001$, 0.01 and 0.1 in Fig. 4.

The percentile values on which the percentile curves in Fig. 5 are based are conditional on individual normalized release (i.e., R) values. Thus, these curves characterize the uncertainty in the probability that specific R values will be exceeded rather than the uncertainty in the location of entire CCDFs. For example, it is inappropriate to conclude that there is a probability of 0.9 that a CCDF produced for a randomly selected element of $\mathcal{S}_{su}$ will fall below the 90th percentile curve. The probability that a CCDF will fall below a specified boundary line (e.g., the boundary line defined in 40 CFR 191.13(a) and illustrated in Fig. 4) can be estimated by generating a sample from $\mathcal{S}_{su}$ as indicated in Eq. (17) and then dividing the number of CCDFs below the boundary line by the sample size. In contrast as shown by the development leading to Eq. (19), connecting the mean exceedance probabilities for individual R values produces the unconditional CCDF discussed in Sect. 3.1.

3.4 CCDF Conditional on Element of $\mathcal{S}_{st}$

The construction of a CCDF conditional on the occurrence of a specific element of $\mathcal{S}_{st}$ is now considered. This case is similar to the case considered in Sect. 3.2 for a CCDF conditional on the occurrence of a specific element of $\mathcal{S}_{su}$. It is useful to first consider the more general case of a CCDF conditional on the occurrence of an arbitrary subset $\mathcal{E}_{st}$ of $\mathcal{S}_{st}$. The corresponding conditional CCDF for normalized release to the accessible environment has the form shown in Eq. (5), where the probability space under consideration is the product space associated with $\mathcal{S}_{st} \times \mathcal{S}_{su}$. As a result, the CCDF is actually conditional on the occurrence of $\mathcal{E}_{st} \times \mathcal{S}_{su}$. Specifically,

$$CCDF(R \mid \mathcal{E}_{st} \times \mathcal{S}_{su}) = \int_{\mathcal{E}_{st} \times \mathcal{S}_{su}} \delta_R[f(\mathbf{x})]\, d(\mathbf{x}) dV \,/ \int_{\mathcal{E}_{st} \times \mathcal{S}_{su}} d(\mathbf{x}) dV, \quad \mathbf{x} = [\mathbf{x}_{st}, \mathbf{x}_{su}]$$

$$= \int_{\mathcal{E}_{st}} \int_{\mathcal{S}_{su}} \delta_R[f(\mathbf{x}_{st}, \mathbf{x}_{su})]\, d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})\, dV_{su}\, dV_{st}$$

$$/ \int_{\mathcal{E}_{st}} \int_{\mathcal{S}_{su}} d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})\, d_{su}(\mathbf{x}_{su})\, dV_{su}\, dV_{st}, \qquad (27)$$

where $CCDF(R \mid \mathcal{E}_{st} \times \mathcal{S}_{su})$ is the probability that a normalized release of size R will be exceeded conditional on the occurrence of $\mathcal{E}_{st} \times \mathcal{S}_{su}$.

To obtain a CCDF conditional on the occurrence of an element $\tilde{\mathbf{x}}_{st}$ of $\mathcal{S}_{st}$, it is necessary to consider the limit of the expression in Eq. (27) as the volumes of sets $\mathcal{E}_{st}$ that contain $\tilde{\mathbf{x}}_{st}$ go to zero (i.e., as $V(\mathcal{E}_{st}) \rightarrow 0$). Given the ratio in Eq. (27), this limit does not have a simple form due to the dependence of $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ and $d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})$ on $\mathbf{x}_{su}$. However, considerable simplification is possible provided there is no relationship between the variables in $\mathbf{x}_{su}$ that affect f and the variables in $\mathbf{x}_{su}$ that affect d_{st}. As discussed in the next paragraph, this is the case in recent PAs for the WIPP.

In recent PAs for the WIPP, the probability space $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$ for subjective uncertainty is itself a product space obtained by combining a probability space $(\mathcal{S}_{su,d}, \mathscr{S}_{su,d}, p_{su,d})$, which characterizes the uncertainty in variables used in the definition of the functions p_{st} and d_{st}, and a probability space $(\mathcal{S}_{su,f}, \mathscr{S}_{su,f}, p_{su,f})$, which characterizes the uncertainty in variables used in the definition of the function f. The elements $\mathbf{x}_{su,d}$ of $\mathcal{S}_{su,d}$ are of the form

$$\mathbf{x}_{su,d} = [BPAREAFR, LAMBDA], \qquad (28)$$

where *BPAREAFR* and *LAMBDA* are defined in Table 1. Thus, $\mathcal{S}_{su,d}$ is a subset of R^2. The distributions indicated in Table 1 provide the information needed to complete the definition of $(\mathcal{S}_{su,d}, \mathscr{S}_{su,d}, p_{su,d})$. Similarly, the elements $\mathbf{x}_{su,f}$ of $\mathcal{S}_{su,f}$ are vectors containing the remaining 43 variables indicated in Table 1 (i.e., $\mathcal{S}_{su,f}$ is a subset of R^{43}) and the indicated distributions in Table 1 provide the information needed to complete the definition of $(\mathcal{S}_{su,f}, \mathscr{S}_{su,f}, p_{su,f})$. As $\mathcal{S}_{su} = \mathcal{S}_{su,d} \times \mathcal{S}_{su,f}$, each element $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$ has the form

$$\mathbf{x}_{su} = [\mathbf{x}_{su,d}, \mathbf{x}_{su,f}] \qquad (29)$$

and is thus a vector from R^{45} as previously noted. Further, the functions f and d_{st} in Eq. (27) are actually of the form $f(\mathbf{x}_{st}, \mathbf{x}_{su,f})$ and $d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su,d})$ rather than $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ and $d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})$. Finally, if $\mathcal{E}_{su,d} \in \mathscr{S}_{su,d}$, $\mathcal{E}_{su,f} \in \mathscr{S}_{su,f}$ and $\mathcal{E}_{su} = \mathcal{E}_{su,d} \times \mathcal{E}_{su,f}$, then

$$p_{su}(\mathcal{E}_{su}) = \int_{\mathcal{E}_{su}} d_{su}(\mathbf{x}_{su})\,dV_{su}$$

$$= \int_{\mathcal{E}_{su,d}} \int_{\mathcal{E}_{su,f}} d_{su,d}(\mathbf{x}_{su,d})\, d_{su,f}(\mathbf{x}_{su,f})\, dV_{su,f}\, dV_{su,d}, \qquad (30)$$

where $d_{su,d}$ and $d_{su,f}$ are the density functions associated with the probability spaces ($\mathcal{S}_{su,d}$, $\mathcal{J}_{su,d}$, $p_{su,d}$) and ($\mathcal{S}_{su,f}$, $\mathcal{J}_{su,f}$, $p_{su,f}$), respectively, and the indicated decomposition in Eq. (30) follows from the assumed independence of the two preceding spaces.

Due to the considerations indicated in the preceding paragraph, the relationship in Eq. (27) is actually of the form

$$CCDF(R \mid \mathcal{E}_{st} \times \mathcal{S}_{su})$$

$$= \int_{\mathcal{E}_{st}} \int_{\mathcal{S}_{su,d}} \int_{\mathcal{S}_{su,f}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su,f})\right] d_{su,f}(\mathbf{x}_{su,f})\, d_{su,d}(\mathbf{x}_{su,d})\, d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su,d})\, dV_{su,f}\, dV_{su,d}\, dV_{st}$$

$$/ \int_{\mathcal{E}_{st}} \int_{\mathcal{S}_{su,d}} \int_{\mathcal{S}_{su,f}} d_{su,f}(\mathbf{x}_{su,f})\, d_{su,d}(\mathbf{x}_{su,d})\, d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su,d})\, dV_{su,f}\, dV_{su,d}\, dV_{st}$$

$$= \int_{\mathcal{E}_{st}} \int_{\mathcal{S}_{su,d}} \int_{\mathcal{S}_{su,f}} \delta_R\left[f(\mathbf{x}_{st}, \mathbf{x}_{su,f})\right] d_{su,f}(\mathbf{x}_{su,f})\, d_{su,d}(\mathbf{x}_{su,d})\, d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su,d})\, dV_{su,f}\, dV_{su,d}\, dV_{st}$$

$$/ \int_{\mathcal{E}_{st}} \int_{\mathcal{S}_{su,d}} d_{su,d}(\mathbf{x}_{su,d})\, d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su,d})\, dV_{su,d}\, dV_{st} \qquad (31)$$

in recent PAs for the WIPP.

The expression in Eq. (31) can now be used to obtain the CCDF for normalized release to the accessible environment conditional on the occurrence of an element $\tilde{\mathbf{x}}_{st}$ of $\mathcal{S}_{st}$. Specifically, with the assumption that $\tilde{\mathbf{x}}_{st} \in \mathcal{E}_{st}$,

$$CCDF(R \mid \{\tilde{\mathbf{x}}_{st}\} \times \mathcal{S}_{su}) = \lim_{V(\mathcal{E}_{st}) \to 0} CCDF(R \mid \mathcal{E}_{st} \times \mathcal{S}_{su})$$

$$= \lim_{V(\mathcal{E}_{st}) \to 0} \left\{ \left[\int_{\mathcal{S}_{su,d}} \int_{\mathcal{S}_{su,f}} \delta_R\left[f(\bar{\mathbf{x}}_{st}, \mathbf{x}_{su,f})\right] d_{su,f}(\mathbf{x}_{su,f})\, d_{su,d}(\mathbf{x}_{su,d})\, d_{st}(\bar{\mathbf{x}}_{st} \mid \mathbf{x}_{su,d})\, dV_{su,f}\, dV_{su,d} \right] V(\mathcal{E}_{st}) \right.$$

$$\left. / \left[\int_{\mathcal{S}_{su,d}} d_{su,d}(\mathbf{x}_{su,d})\, d_{st}(\hat{\mathbf{x}}_{st} \mid \mathbf{x}_{su,d})\, dV_{su,d} \right] V(\mathcal{E}_{st}) \right\}$$

[from Eq. (31) by mean value theorem with $\bar{\mathbf{x}}_{st}, \hat{\mathbf{x}}_{st} \in \mathcal{E}_{st}$]

$$= \lim_{V(\mathcal{E}_{st})\to 0} \left\{ \int_{\mathcal{S}_{su,f}} \delta_R\left[f\left(\tilde{\mathbf{x}}_{st}, \mathbf{x}_{su,f}\right)\right] d_{su,f}\left(\mathbf{x}_{su,f}\right) dV_{su,f} \right\}$$

$$\bullet \left\{ \frac{\int_{\mathcal{S}_{su,d}} d_{su,d}\left(\mathbf{x}_{su,d}\right) d_{st}\left(\tilde{\mathbf{x}}_{st} | \mathbf{x}_{su,d}\right) dV_{su,d}}{\int_{\mathcal{S}_{su,d}} d_{su,d}\left(\mathbf{x}_{su,d}\right) d_{st}\left(\hat{\mathbf{x}}_{st} | \mathbf{x}_{su,d}\right) dV_{su,d}} \right\}$$

$$= \int_{\mathcal{S}_{su,f}} \delta_R\left[f\left(\tilde{\mathbf{x}}_{st}, \mathbf{x}_{su,f}\right)\right] d_{su,f}\left(\mathbf{x}_{su,f}\right) dV_{su,f}, \tag{32}$$

provided the functions involved are "reasonably" behaved. The representation for $CCDF\left(R|\{\tilde{\mathbf{x}}_{st}\}\times\mathcal{S}_{su}\right)$ in Eq. (32) gives the probability that a normalized release of size R will be exceeded conditional on the occurrence of the element $\tilde{\mathbf{x}}_{st}$ of $\mathcal{S}_{st}$.

As is the case for all integrals discussed in this presentation, the WIPP PA does not evaluate the integral in Eq. (32) directly. Rather, an approximation procedure is used. Specifically,

$$CCDF\left(R|\{\mathbf{x}_{st}\}\times\mathcal{S}_{su}\right) \doteq \sum_{k=1}^{nLHS} \delta_R\left[f\left(\mathbf{x}_{st}, \mathbf{x}_{su,f,k}\right)\right] / nLHS, \tag{33}$$

where, in consistency with the notation used in Eq. (32), the elements of the Latin hypercube sample indicated in Eq. (17) are assumed to be of the form

$$\mathbf{x}_{su,k} = \left[\mathbf{x}_{su,d,k}, \mathbf{x}_{su,f,k}\right]. \tag{34}$$

The 1991 WIPP PA evaluated CCDFs of the form defined in Eq. (33) for 10 elements of $\mathcal{S}_{st}$: single drilling intrusions at 1,000, 3,000, 5,000, 7,000 and 9,000, yr and E1E2-type drilling intrusions at 1,000, 3,000, 5,000, 7,000 and 9,000 yr, where an E1E2-type intrusion involves two or more boreholes penetrating the same waste panel, with at least one intrusion penetrating a pressurized brine pocket and at least one intrusion not penetrating a pressurized brine pocket. The resultant CCDFs for groundwater transport to the accessible environment are shown in Fig. 7. As illustrated in Fig. 8, box plots are often used in the WIPP PA to summarize distributions of the form appearing in Fig. 7 due to their greater compactness and legibility.

If $\mathbf{x}_{su}$ does not have the decomposition in Eq. (29), the outcome of evaluating the limit in Eq. (32) is

$$CCDF\left(R|\{\tilde{\mathbf{x}}_{st}\}\times\mathcal{S}_{su}\right)$$

$$= \left[\int_{\mathcal{S}_{su}} \delta_R\left[f\left(\tilde{\mathbf{x}}_{st}, \mathbf{x}_{su}\right)\right] d_{st}\left(\tilde{\mathbf{x}}_{st}|\mathbf{x}_{su}\right) d_{su}\left(\mathbf{x}_{su}\right) dV_{su}\right] / \left[\int_{\mathcal{S}_{su}} d_{st}\left(\tilde{\mathbf{x}}_{st}|\mathbf{x}_{su}\right) d_{su}\left(\mathbf{x}_{su}\right) dV_{su}\right]$$

$$= \int_{\mathcal{S}_{su}} \delta_R\left[f\left(\tilde{\mathbf{x}}_{st}, \mathbf{x}_{su}\right)\right] d_{su}\left(\mathbf{x}_{su}|\tilde{\mathbf{x}}_{st}\right) dV_{su}, \tag{35}$$

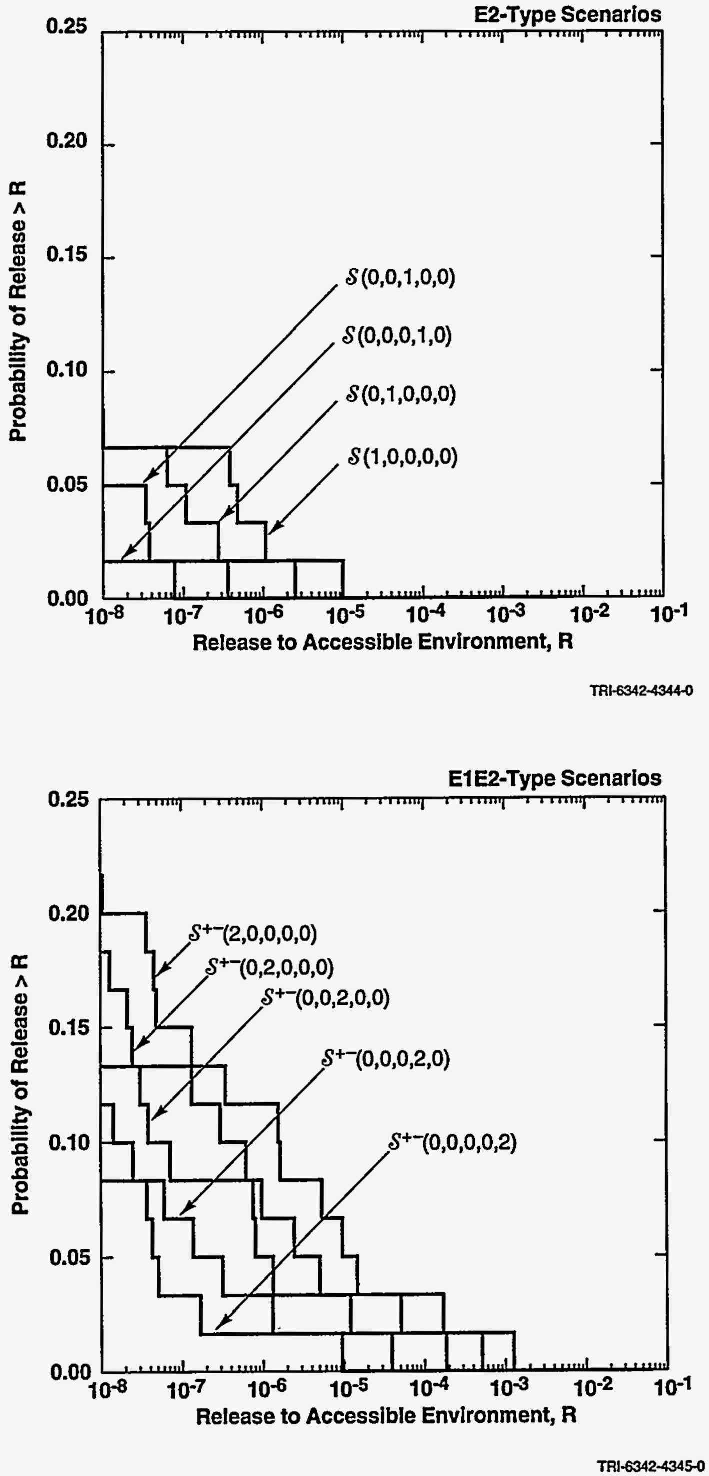

Fig. 7. Complementary cumulative distribution functions for normalized release to the accessible environment due to groundwater transport conditional on the occurrence of individual elements of $\mathcal{S}_{st}$. The upper plot frame contains CCDFs for single intrusions at 1000, 3000, 5000 and 7000 yrs (i.e., for scenarios $\mathcal{S}$(1,0,0,0,0), $\mathcal{S}$(0,1,0,0,0), $\mathcal{S}$(0,0,1,0,0), $\mathcal{S}$(0,0,0,1,0) in the notation used in the 1991 WIPP PA); a single intrusion at 9000 yr (i.e., scenario $\mathcal{S}$(0,0,0,0,1)) resulted in no release. The lower plot frame contains CCDFs for E1E2-type drilling intrusions at 1000, 3000, 5000, 7000 and 9000 yrs (i.e., for scenarios $\mathcal{S}^{+-}$(2,0,0,0,0), ... , $\mathcal{S}^{+-}$(0,0,0,0,2)).

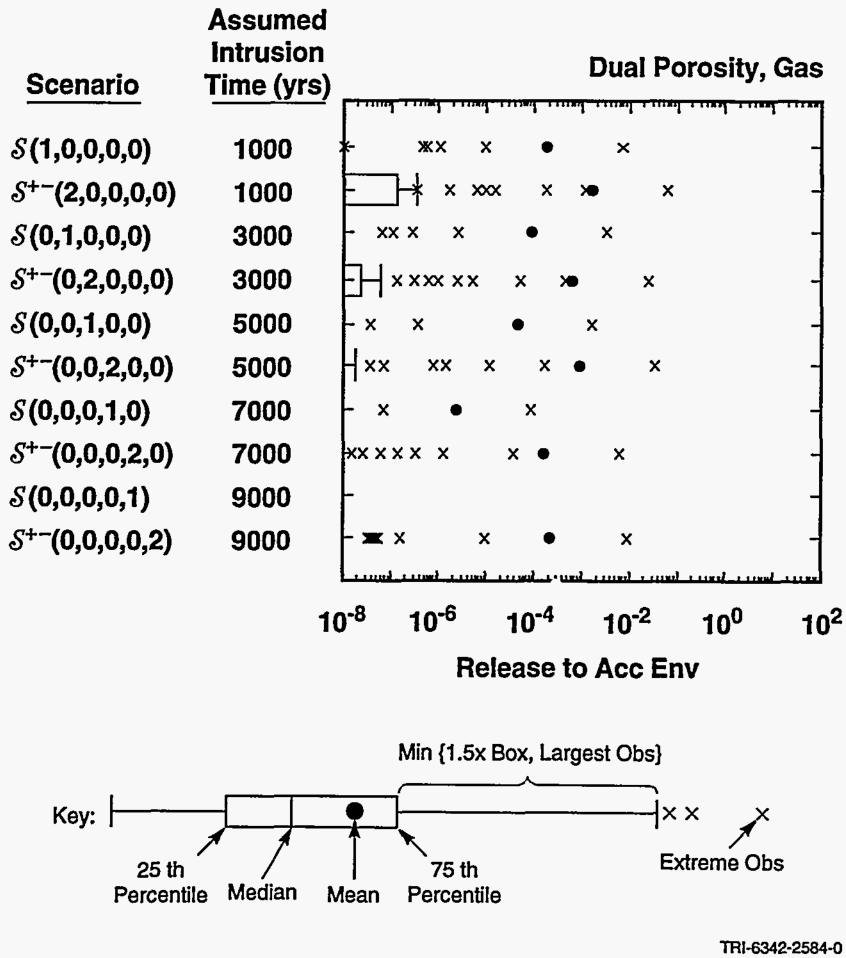

Fig. 8. Alternative summary of CCDFs in Fig. 7 with box plots (Ref. 24, Fig. 4.4-1; Ref. 49, Fig. 10).

where $d_{su}(\mathbf{x}_{su}|\tilde{\mathbf{x}}_{st})$ is the density function for $\mathbf{x}_{su}$ conditional on the occurrence of $\tilde{\mathbf{x}}_{st}$ (Table 2). If a sample from $\mathcal{S}_{su}$ of the form indicated in Eq. (17) is used, then the CCDF in Eq. (35) can be approximated by

$$CCDF\left(R|\{\tilde{\mathbf{x}}_{st}\}\times\mathcal{S}_{su}\right)\doteq\left[\sum_{k=1}^{nLHS}\delta_R\left[f\left(\tilde{\mathbf{x}}_{st},\mathbf{x}_{su,k}\right)\right]d_{st}\left(\tilde{\mathbf{x}}_{st}|\mathbf{x}_{su,k}\right)\right]/\left[\sum_{k=1}^{nLHS}d_{st}\left(\tilde{\mathbf{x}}_{st}|\mathbf{x}_{su,k}\right)\right], \tag{36}$$

which is equivalent to use of the reweighting procedure proposed by Iman and Conover.[54]

3.5 Alternate Construction of Unconditional CCDF on Product Space $\mathcal{S}_{st}\times\mathcal{S}_{su}$

The unconditional quantity *CCDF(R)* was obtained in Eq. (16) by integrating over the probability space associated with $\mathcal{S}=\mathcal{S}_{st}\times\mathcal{S}_{su}$. As discussed in Sect. 3.2, *CCDF(R)* is the mean of CCDFs conditional on individual elements of $\mathcal{S}_{su}$, with this mean being calculated with respect to $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. Eqs. (18) and (24) show that an approximation to *CCDF(R)* can be constructed by first approximating CCDFs conditional on elements of $\mathcal{S}_{su}$ obtained by random or Latin hypercube sampling and then vertically averaging these CCDFs.

An alternate approximation procedure for *CCDF(R)* is to calculate CCDFs conditional on elements of $\mathcal{S}_{st}$ as discussed in Sect. 3.4 and then vertically average these CCDFs over $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$. Formally,

$$\begin{aligned}CCDF(R)&=\int_{\mathcal{S}_{st}}CCDF\left(R|\{\mathbf{x}_{st}\}\times\mathcal{S}_{su}\right)d_{st}(\mathbf{x}_{st})\,dV_{st}\ \left[\text{see Table 2 for definition of } d_{st}(\mathbf{x}_{st})\right]\\
&=\int_{\mathcal{S}_{st}}\int_{\mathcal{S}_{su}}\delta_R\left[f\left(\mathbf{x}_{st},\mathbf{x}_{su}\right)\right]d_{st}\left(\mathbf{x}_{st}|\mathbf{x}_{su}\right)d_{su}\left(\mathbf{x}_{su}\right)dV_{su}\,dV_{st}\ \left[\text{from Eq. (35)}\right]\\
&=\int_{\mathcal{S}_{su}}\int_{\mathcal{S}_{st}}\delta_R\left[f\left(\mathbf{x}_{st},\mathbf{x}_{su}\right)\right]d_{st}\left(\mathbf{x}_{st}|\mathbf{x}_{su}\right)d_{su}\left(\mathbf{x}_{su}\right)dV_{st}\,dV_{su},\end{aligned} \tag{37}$$

which is the same outcome as in Eq. (16).

An approximation to *CCDF(R)* is obtained by subdividing $\mathcal{S}_{st}$ into a sequence $\mathcal{S}_{st,i}$, $i = 1, 2, ..., nS$, of disjoint subsets. Specifically,

$$\begin{aligned}CCDF(R)&=\sum_{i=1}^{nS}\int_{\mathcal{S}_{st,i}}CCDF\left(R|\{\mathbf{x}_{st}\}\times\mathcal{S}_{su}\right)d_{st}\left(\mathbf{x}_{st}\right)dV_{st}\ \left[\mathcal{S}_{st}=\cup_i\mathcal{S}_{st,i},\ \mathcal{S}_{st,i}\cap\mathcal{S}_{st,j}=\phi\ \text{ for } i\neq j\right]\\
&=\sum_{i=1}^{nS}\left\{CCDF\left(R|\{\mathbf{x}_{st,i}\}\times\mathcal{S}_{su}\right)\right\}\left\{\int_{\mathcal{S}_{st,i}}d_{st}\left(\mathbf{x}_{st}\right)dV_{st}\right\}\\
&\qquad\left[\text{by generalized mean value of theorem with } \mathbf{x}_{st,i}\in\mathcal{S}_{st,i}\right]\end{aligned}$$

$$= \sum_{i=1}^{nS} \left\{ CCDF\left(R \mid \left\{\mathbf{x}_{st,i}\right\} \times \mathcal{S}_{su}\right)\right\} \left\{ \int_{\mathcal{S}_{su}} \left[\int_{\mathcal{S}_{st,i}} d_{st}\left(\mathbf{x}_{st} \mid \mathbf{x}_{su}\right) dV_{st} \right] d_{su}\left(\mathbf{x}_{su}\right) dV_{su} \right\}, \quad (38)$$

[from definition of $d_{st}(\mathbf{x}_{st})$ in Table 2]

where in the final equality

$$p\left(\mathcal{S}_{st,i} \mid \mathbf{x}_{su}\right) = \int_{\mathcal{S}_{st,i}} d_{st}\left(\mathbf{x}_{st} \mid \mathbf{x}_{su}\right) dV_{st} \quad (39)$$

is the probability of $\mathcal{S}_{st,i}$ given $\mathbf{x}_{su}$ and

$$p\left(\mathcal{S}_{st,i}\right) = \int_{\mathcal{S}_{su}} p\left(\mathcal{S}_{st,i} \mid \mathbf{x}_{su}\right) d_{su}\left(\mathbf{x}_{su}\right) dV_{su} \quad (40)$$

is the expected value of $p(\mathcal{S}_{st,i} \mid \mathbf{x}_{su})$ over $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$.

If a sample from $\mathcal{S}_{su}$ of the form indicated in Eq. (17) is used, then the results in Eqs. (36) and (38) can be combined to obtain the following approximation to $CCDF(R)$:

$$CCDF(R) \doteq \sum_{i=1}^{nS} \left\{ \left[\sum_{k=1}^{nLHS} \delta_R\left[f\left(\mathbf{x}_{st,i}, \mathbf{x}_{su,k}\right)\right] d_{st}\left(\mathbf{x}_{st,i} \mid \mathbf{x}_{su,k}\right) \right] \Big/ \left[\sum_{k=1}^{nLHS} d_{st}\left(\mathbf{x}_{st,i} \mid \mathbf{x}_{su,k}\right) \right] \right\}_1$$

$$\bullet \left\{ \sum_{k=1}^{nLHS} \left[\int_{\mathcal{S}_{st,i}} d_{st}\left(\mathbf{x}_{st} \mid \mathbf{x}_{su,k}\right) dV_{st} \right] \Big/ nLHS \right\}_2, \quad (41)$$

where $\{\sim\}_1$ is an approximation to a CCDF over subjective uncertainty conditional on the occurrence of an element $\mathbf{x}_{st,i}$ of $\mathcal{S}_{st,i}$ and $\{\sim\}_2$ is an approximation to the expected value over subjective uncertainty for the probability of $\mathcal{S}_{st,i}$. If $\mathbf{x}_{su}$ has the decomposition indicated in Eq. (29) and a sample of the form in Eq. (34) is used, then the results in Eqs. (33) and (38) can be combined to obtain

$$CCDF(R) \doteq \sum_{i=1}^{nS} \left\{ \sum_{k=1}^{nLHS} \delta_R\left[f\left(\mathbf{x}_{st,i}, \mathbf{x}_{su,f,k}\right)\right] \Big/ nLHS \right\}_1 \left\{ \sum_{k=1}^{nLHS} \left[\int_{\mathcal{S}_{st,i}} d_{st}\left(\mathbf{x}_{st} \mid \mathbf{x}_{su,k}\right) dV_{st} \right] \Big/ nLHS \right\}_2, \quad (42)$$

where $\{\sim\}_1$ and $\{\sim\}_2$ have the same interpretation as in Eq. (41).

The approximations to $CCDF(R)$ in Eqs. (41) and (42) both involve a construction procedure of the form indicated in Fig. 9, with CCDFs conditional on the occurrence of individual elements of $\mathcal{S}_{st}$ being constructed and then vertically averaged to obtain an approximation to $CCDF(R)$. The first term (i.e., $\{\sim\}_1$) in Eqs. (41) and (42) is an approximation to the conditional CCDFs (i.e., to $CCDF\left(R \mid \left\{\mathbf{x}_{st,i}\right\} \times \mathcal{S}_{su}\right)$ in Fig. 9. The second term (i.e., $\{\sim\}_2$) in Eqs. (41) and (42) is an approximation to the probability (i.e., to $p(\mathcal{S}_{st,i})$) of the subsets $\mathcal{S}_{st,i}$ of $\mathcal{S}_{st}$ on which the

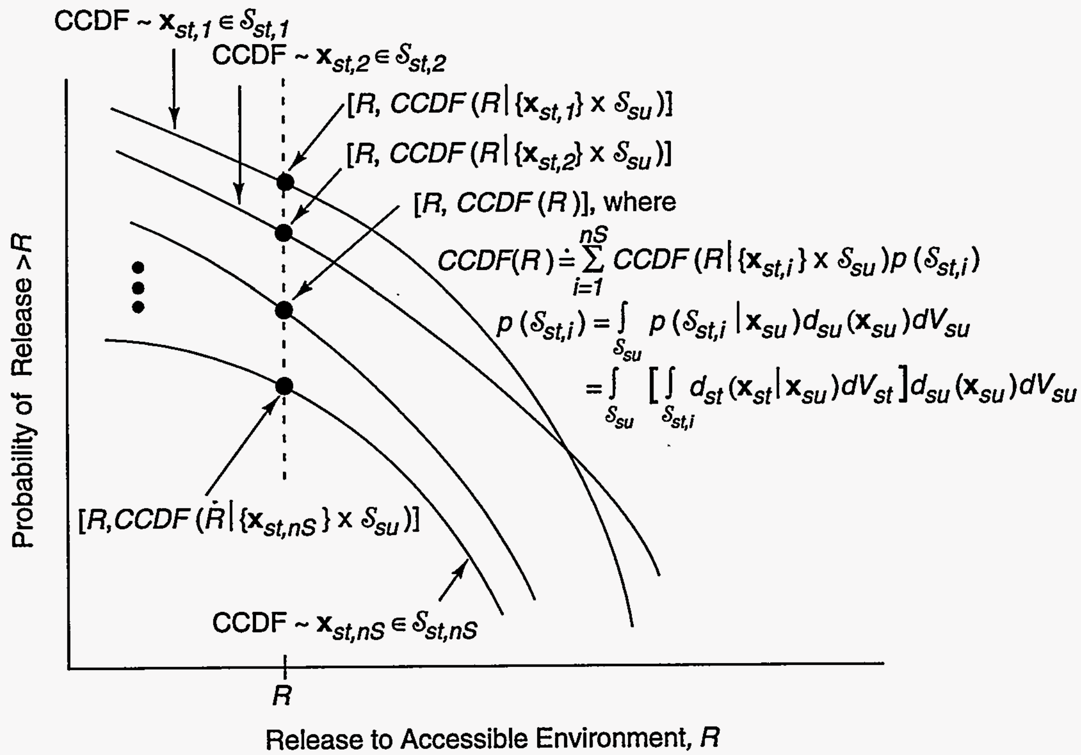

Fig. 9. Construction of Unconditional CCDF on $\mathcal{S}_{st} \times \mathcal{S}_{su}$ (i.e., $CCDF(R)$) by Vertically Averaging CCDFs Conditional on the Occurrence of Elements of $\mathcal{S}_{st}$.

construction of $CCDF(R)$ is based. The summation in Eqs. (41) and (42) produces an approximation to the CCDF labeled $CCDF(R)$ in Fig. 9.

Although Eqs. (41) and (42) approximate $p(\mathcal{S}_{st,i})$ in the same manner, the approximations to $CCDF\left(R|\{\mathbf{x}_{st,i}\}\times \mathcal{S}_{su}\right)$ are different. The independence of variables that affect $f(\mathbf{x}_{st}, \mathbf{x}_{su,f})$ and $d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su,d})$ in Eq. (42) allows the approximation to $CCDF\left(R|\{\mathbf{x}_{st,i}\}\times \mathcal{S}_{su}\right)$ to be constructed directly from the values of $f(\mathbf{x}_{st,i}, \mathbf{x}_{su,f,k})$ calculated for the sample elements $\mathbf{x}_{su,f,k}$, k=1, 2, ..., $nLHS$. In contrast, the corresponding lack of independence for Eq. (41) requires the inclusion of a weighting term in the approximation to $CCDF\left(R|\{\mathbf{x}_{st,i}\}\times \mathcal{S}_{su}\right)$.

The approximation procedure in Eq. (42) has often been proposed for estimating $CCDF(R)$, with there typically being no uncertainty in the probability for subsets $\mathcal{S}_{st,i}$ of $\mathcal{S}_{st}$.[55-59] However, there are two disadvantages to the use of Eq. (42). First, by directly constructing $CCDF(R)$ from CCDFs conditional on elements of $\mathcal{S}_{st}$, the uncertainty associated with $(\mathcal{S}_{su}, \mathcal{s}_{su}, p_{su})$ that leads to multiple possible CCDFs for comparison with 40 CFR 191.13 is obscured. Second, when many subsets $\mathcal{S}_{st,i}$ of $\mathcal{S}_{st}$ are in use, this procedure can become computationally unwieldy. For example, nS exceeded 10^6 in the construction of some of the CCDFs in Fig. 4 (see Ref. 40, Table 2). In addition, the use of Eq. (41) when the variables associated with $(\mathcal{S}_{su}, \mathcal{s}_{su}, p_{su})$ that affect $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ and $d_{st}(\mathbf{x}_{st} | \mathbf{x}_{su})$

are not independent requires the inclusion of weights with the calculated results for individual sample elements. The requirements for these weights is the reason why the approximation in Eq. (20) of Ref. 15 will not, in general, produce the same CCDF as the approximations in Eqs. (19) and (41); however, it does produce the same CCDF as Eq. (42) when the variables that affect $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ and $d_{st}(\mathbf{x}_{st} \mid \mathbf{x}_{su})$ are independent.

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4. Discussion

As evidenced by the extensive discussion in Refs. 1-20, much interest exists in the treatment of uncertainty in PAs for complex systems. Indeed, the incorporation of uncertainty into the outcomes of an analysis is the essence of a PA for a complex system. However, appropriately drawing a distinction between the uncertainty that arises because the system can behave in many different ways (i.e., stochastic uncertainty) and the uncertainty that arises from a lack of knowledge on the part of the analysts conducting the PA (i.e., subjective uncertainty) remains an area of considerable confusion.

This presentation describes and illustrates a formal approach to representing the uncertainty in a PA for a complex system in which a probability space $(\mathcal{S}_{st}, \mathcal{S}_{st}, p_{st})$ is used to characterize stochastic uncertainty, a probability space $(\mathcal{S}_{su}, \mathcal{S}_{su}, p_{su})$ is used to characterize subjective uncertainty, and the models used in the PA are functions (i.e., random variables) defined on the product space associated with $(\mathcal{S}_{st}, \mathcal{S}_{st}, p_{st})$ and $(\mathcal{S}_{su}, \mathcal{S}_{su}, p_{su})$. Initially, this can sound very complicated. However, this structure produces a relatively simple conceptual description of a PA into which the many individual components of the PA can be placed and leads naturally to the actual calculations that are performed within a PA.

The development of the probability space $(\mathcal{S}_{st}, \mathcal{S}_{st}, p_{st})$ is central to all PAs. For example, the fault and event tree techniques that play an important role in many large analyses can be viewed as algorithms for developing, or at least approximating, $(\mathcal{S}_{st}, \mathcal{S}_{st}, p_{st})$. An inevitably-posed question in every large PA involves completeness; specifically "Did the PA consider everything that could occur in the system under study?". What this question is actually asking is whether or not the sample space $\mathcal{S}_{st}$ was appropriately defined. Another activity that arises in one form or another in all PAs is scenario development and involves the selection of subsets of $\mathcal{S}_{st}$ for consideration in the PA. Typically, scenarios are elements of $\mathcal{S}_{st}$ for which probabilities are determined and consequence calculations are carried out. Thus, scenario development can be viewed as the determination of sets in $\mathcal{S}_{st}$ for inclusion in the PA. Finally, p_{st} must be developed if probabilistic statements are to be made about occurrences in the system under study. An important point that should be recognized is that, although probabilities are determined for subsets of $\mathcal{S}_{st}$, consequence calculations are performed for individual elements of $\mathcal{S}_{st}$. Thus, an important consideration in scenario development is to obtain subsets of $\mathcal{S}_{st}$ that are reasonably homogeneous so that a calculation performed for an arbitrary element of $\mathcal{S}_{st}$ in a scenario will produce results that are reasonably close to what would be obtained for any other element of $\mathcal{S}_{st}$ associated with the scenario.

A clear conceptual model for a PA is very important. At the same time, it is important to recognize how computational practice diverges from this conceptual model. For example, in most large analyses $\mathcal{S}_{st}$, $\mathcal{S}_{st}$ and p_{st} are never fully developed. Rather, fault and event tree techniques or some other construction procedure are used to develop a collection of disjoint sets that spans $\mathcal{S}_{st}$. The nature of $\mathcal{S}_{st}$ is then inferred from these sets, and p_{st} is defined only for these sets. Thus, although a probability space $(\mathcal{S}_{st}, \mathcal{S}_{st}, p_{st})$ for stochastic uncertainty underlies the analysis, this space is never known completely. Rather, enough information about $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ is developed to allow the analysis to be performed but a complete construction of $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ is not carried out.

Much of what is done in a PA involves integrations performed with the probability spaces $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ and $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. Integration of suitably defined functions over $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ leads to the CCDFs that are typically presented as the outcomes of PAs for complex systems. For most systems, integration procedures based on importance sampling or Monte Carlo techniques are used. In the example contained in this presentation, an integration procedure based on importance sampling was used to estimate the CCDF specified in the EPA's regulation 191.13(a) for the geologic disposal of radioactive waste. This CCDF could also have been estimated with Monte Carlo procedures.[60] The fault tree and event tree techniques used in many large analyses to develop scenarios can also be viewed as algorithms to define importance sampling procedures for integration over $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$. Importance sampling procedures are often used because they provide a way to assure the inclusion of low probability but possibly high consequence subsets of $\mathcal{S}_{st}$ in the analysis. What are rather lightly referred to as "suitably defined functions" at the beginning of this paragraph are often sequences of complex computer programs. Thus, the closed form evaluation of integrals is typically not a possibility in PAs for complex systems.

The probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ enters a PA when it is desired to express the analysts' confidence in the outcomes of the study. Often, $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ is developed at least in part through an expert review process in which distributions are developed to characterize the state of knowledge uncertainty in individual variables used in the analyses. Taken collectively, these distributions then define $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. In the example contained in this presentation, the uncertainty characterized by $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ leads to an assessment of the "reasonable expectation" called for in the EPA's regulation 191.13(b). As for $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$, the implications of the uncertainty characterized by $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ must be determined by numerical integration procedures. Possibilities include the discrete probability method[61] and Monte Carlo procedures based on simple random sampling or Latin hypercube sampling. The example contained in this presentation and also the NUREG-1150 probabilistic risk assessments[13,62] used Latin hypercube sampling because of its efficient stratification properties.

The integration procedures indicated in the two preceding paragraphs can also be viewed as the outcome of experimental designs applied to $\mathcal{S}_{st}$ and $\mathcal{S}_{su}$. Thus, the subdivision of $\mathcal{S}_{st}$ into scenarios (i.e.., elements of $\mathcal{J}_{st}$) is an experimental design based on importance sampling. Similarly, the use of Monte Carlo procedures based on simple random sampling or Latin hypercube sampling can be viewed as generating random designs.

The Kaplan/Garrick ordered triple representation for risk[2] provides a useful way to view the structure of a PA that is consistent with the ideas discussed in this presentation. In the Kaplan/Garrick representation, risk is represented by a set $\mathcal{R}$ of the form

$$\mathcal{R} = \{(\mathcal{S}_i, pS_i, \mathbf{cS}_i), i = 1, \ldots, nS\}, \tag{43}$$

where $\mathcal{S}_i$ is a set of similar occurrences, pS_i is the probability that an occurrence in the set $\mathcal{S}_i$ will take place, $\mathbf{cS}_i$ is a vector of consequence associated with $\mathcal{S}_i$, nS is the number of sets selected for consideration, the sets $\mathcal{S}_i$ have no occurrences in common, and $\cup_i \mathcal{S}_i$ contains everything that could occur in the system under consideration. In the context of the probability space $(\mathcal{S}_{st}, \mathscr{S}_{st}, p_{st})$, the $\mathcal{S}_i$ are elements of $\mathscr{S}_{st}$, the sample space $\mathcal{S}_{st}$ is equal to $\cup_i \mathcal{S}_i$, and pS_i is equal to $p_{st}(\mathcal{S}_i)$. Further, $\mathbf{cS}_i$ is obtained by evaluating a function f for a suitably selected element of $\mathcal{S}_i$; another possibility is that $\mathbf{cS}_i$ is the expected value of f on $\mathcal{S}_i$ but this usage is less common. Thus, the Kaplan/Garrick ordered triple representation for risk is simply a way to develop the CCDFs for the probability space $(\mathcal{S}_{st}, \mathscr{S}_{st}, p_{st})$ and an associated function f defined on $\mathcal{S}_{st}$.

Subjective uncertainty enters into the risk representation in Eq. (43) through the recognition that $\mathcal{R}$ is actually a function of the form

$$\mathcal{R}(\mathbf{x}) = \left\{\left[\mathcal{S}_i(\mathbf{x}), pS_i(\mathbf{x}), \mathbf{cS}_i(\mathbf{x})\right], i = 1, \ldots, nS(\mathbf{x})\right\}, \quad (44)$$

where

$$\mathbf{x} = \left[x_1, x_2, \ldots, x_{nV}\right] \quad (45)$$

is a vector of imprecisely known inputs required in the analysis. Lack of knowledge about $\mathbf{x}$ is subjective uncertainty and is characterized by the probability space $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$. In practice, $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$ is defined by a sequence of distributions

$$D_1, D_2, \ldots, D_{nV} \quad (46)$$

for the individual elements x_j of $\mathbf{x}$. The effect of this uncertainty is typically characterized by generating a random or Latin hypercube sample

$$\mathbf{x}_k, k = 1, 2, \ldots, nK, \quad (47)$$

of size nK according to the distributions in Eq. (46) and then evaluating

$$\mathcal{R}(\mathbf{x}_k) = \left\{\left[\mathcal{S}_i(\mathbf{x}_k), pS_i(\mathbf{x}_k), \mathbf{cS}_i(\mathbf{x}_i)\right], i = 1, \ldots, nS(\mathbf{x}_k)\right\} \quad (48)$$

for $k = 1, 2, \ldots, nK$. The preceding procedure leads to representations of uncertainty of the form shown in Figs. 4-7 and is equivalent to integrating over the probability space $(\mathcal{S}_{su}, \mathscr{S}_{su}, p_{su})$ as discussed in this presentation.

An often contentious point that arises in many PAs is whether or not it is meaningful to have a "probability of a probability." Such a probability arises quite naturally when product spaces are considered. As discussed in Sect. 3.3 and illustrated in Fig. 6, a probability can arise from one probability space (e.g., $(\mathcal{S}_{st}, \mathscr{S}_{st}, p_{st})$ in this presentation) and a distribution for this probability can arise from another probability space (e.g., $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ in this presentation).

A phrase often used in conjunction with PAs for complex systems is "uncertainty and sensitivity analysis." Uncertainty analysis involves determining the uncertainty in analysis outcomes that derives from uncertainty with respect to the correctness of the assumptions used in the analysis. In the terminology of this presentation, uncertainty analysis is an investigation of the effects of subjective uncertainty. Indeed, the primary purpose of this presentation is to provide a formal description of uncertainty analysis in which the dependent variable of interest is a CCDF that results from stochastic uncertainty. Sensitivity analysis involves determining the effects of the uncertainty in individual variables on various analysis outcomes of interest (e.g., the probability of exceeding a given consequence value).[63] Although not emphasized in this presentation, sensitivity analysis typically involves determining the effects of individual variables associated with the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ on either a function f evaluated at a specific point in $\mathcal{S}_{st}$ (e.g., see Ref. 49, Tables IX, X, XI) or an exceedance probability that results from integrating f over $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ (e.g., see Ref. 49, Figs. 27, 28). The modifier "typically" is used in the preceding sentence because it is also possible, though less commonly done, to use sensitivity analysis techniques to investigate the effects of the variability associated with $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ on predicted quantities of interest.

The division of uncertainty into stochastic uncertainty and subjective uncertainty greatly helps in the organization of a large analysis. At times it is argued that this distinction is artificial. However, when the actual computational implementation of an analysis must be confronted, the necessary distinctions are usually apparent. When these distinctions are not immediately apparent, evaluating them forces the analysts to come to grips with the nature of the system that they are studying and the analysis that they are conducting. Even if there is doubt as to how an uncertainty should be classified, the use of a formal structure to describe the analysis should leave no doubt as to how this uncertainty was actually treated. There is nothing wrong with differing views on how an analysis should be conducted and uncertainty treated within the analysis. What is unacceptable is to be unable to determine what was done after an analysis is completed.

This presentation has described a paradigm for the description and organization of a PA for a complex system. In this paradigm, a PA involves three basic components: a probability space $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ for stochastic uncertainty, a probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ for subjective uncertainty, and a function defined on the product space associated with $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ and $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$. All of the basic results used in expressing the outcomes of a PA can be described in terms of these three components. The formalism associated with this paradigm is certainly not for presentation to all groups that may be involved in or interested in a given PA. However, there should be a core of individuals associated with any PA who have a clear conceptual understanding of the organization of the analysis. These individuals can then assure that the treatment of uncertainty and the modeling of physical processes is consistent with this organization and that analysis results are presented in a way that properly communicates what was done in the analysis. The structure described and illustrated in this presentation provides a basis for such an understanding.

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