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Conceptual Structure of the 1996 Performance Assessment for the Waste Isolation Pilot Plant

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Abstract

The conceptual structure of the 1996 performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP) is described. This structure involves three basic entities (EN1, EN2, EN3): (i) EN1, a probabilistic characterization of the likelihood of different futures occurring at the WIPP site over the next 10,000 yr, (ii) EN2, a procedure for estimating the radionuclide releases to the accessible environment associated with each of the possible futures that could occur at the WIPP site over the next 10,000 yr, and (iii) EN3, a probabilistic characterization of the uncertainty in the parameters used in the definition of EN1 and EN2. In the formal development of the 1996 WIPP PA, EN1 is characterized by a probability space ($\mathcal{S}_{st}$, $\mathcal{S}_{st}$, p_{st}) for stochastic (i.e., aleatory) uncertainty; EN2 is characterized by a function f that corresponds to the models and associated computer programs used to estimate radionuclide releases; and EN3 is characterized by a probability space ($\mathcal{S}_{su}$, $\mathcal{S}_{su}$, p_{su}) for subjective (i.e., epistemic) uncertainty. A high-level overview of the 1996 WIPP PA and references to additional sources of information are given in the context of ($\mathcal{S}_{st}$, $\mathcal{S}_{st}$, p_{st}), f and ($\mathcal{S}_{su}$, $\mathcal{S}_{su}$, p_{su}).

Key Words: Aleatory uncertainty, complementary cumulative distribution function, compliance certification application, epistemic uncertainty, Latin hypercube sampling, Monte Carlo, performance assessment, radioactive waste, risk, stochastic uncertainty, subjective uncertainty, transuranic waste, Waste Isolation Pilot Plant, 40 CFR 191, 40 CFR 194.

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1. Introduction

This article provides an overview of the conceptual structure of the 1996 performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP) and references to additional articles that describe the computational implementation of this structure. In turn, the 1996 WIPP PA provides the primary numerical results used in the 1996 compliance certification application (CCA) by the U.S. Department of Energy (DOE) to the U.S. Environmental Protection Agency (EPA) for the certification of the WIPP for the disposal of transuranic (TRU) waste.[1]

Performance assessment for the WIPP began shortly after the EPA promulgated its standard for the geologic (i.e., deep underground) disposal of radioactive waste, *Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* (40 CFR 191).[2, 3] In particular, PAs were carried out for the WIPP in 1989 (Refs. 4 - 6), 1990 (Ref. 7), 1991 (Ref. 8), and 1992 (Ref. 9), with summaries of the 1991 and 1992 PAs available in the journal literature.[10-12] In general, each PA was more sophisticated than its predecessors as more insights were gained about the WIPP and the appropriate organization of a PA for the WIPP (see Ref. 13 for a history of the development of the WIPP).

A system prioritization methodology (SPM) was applied to the WIPP in 1994 (Refs. 14 - 16) and 1995 (Refs. 17 - 19). The SPM was a specialized PA intended to provide guidance to the WIPP project on experimental programs and design modifications to support as part of the DOE's development of the WIPP.

The conceptual structure of the 1996 WIPP PA emerged from insights gained in the earlier analyses and also from the requirements imposed by the EPA's standard for the geologic disposal of radioactive waste.[20, 21] Preliminary descriptions of this structure appear in a sequence of conference papers prepared at various points in the development of the 1996 WIPP PA (Refs. 22 - 24). The conceptual structure of the 1996 WIPP PA is also covered in varying levels of detail in several recent journal articles[25-27] and is repeated here as a convenience for the readers of the special issue of *Reliability Engineering and System Safety* describing the 1996 WIPP PA, of which this article is a part. Inclusion of this material in the special issue facilitates describing the 1996 WIPP PA and identifying the articles in the issue that provide detailed information on the individual parts of the analysis.

This article derives from Chapt. 2 of Ref. 28 and is organized as follows. First, a brief overview of the EPA regulations that influence the conceptual structure of the 1996 WIPP PA is given (Sect. 2). Then, the three basic conceptual entities that underlie the PA are discussed: a probabilistic characterization of what could occur at the WIPP over the next 10,000 yr (Sect. 3); a procedure for estimating radionuclide releases to the accessible environment associated with each of the possible futures that could occur at the WIPP over the next 10,000 yr (Sect. 4); and a probabilistic characterization of the uncertainty present in the characterizations of the two preceding entities (Sect. 5). A discussion of the 1996 WIPP PA in the context of other analyses for complex systems is provided (Sect. 6), and finally, the article ends with a concluding discussion (Sect. 7).

2. Regulatory Requirements (Adapted from Sect. 2, Ref. 26)

The conceptual structure of the 1996 PA for the WIPP derives from the regulatory requirements imposed on this facility.[20, 21, 29] The primary regulation determining this structure is the U.S. EPA's standard for the geologic disposal of radioactive waste (40 CFR 191). The following is the central requirement in 40 CFR 191 and the primary determinant of the conceptual structure of the 1996 WIPP PA (p. 38086, Ref. 2):

> § 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) refers to "quantities calculated according to Table 1 (Appendix A)," which means a normalized radionuclide release to the accessible environment based on the type of waste being disposed of, the initial waste inventory, and the release that takes place (App. A, Ref. 2). Table 1 (Appendix A) specifies allowable releases (i.e., release limits) for individual radionuclides and is reproduced as Table 1 of this presentation. The WIPP is intended for transuranic waste, which is defined to be "waste containing more than 100 nanocuries of alpha-emitting transuranic isotopes, with half-lives greater than twenty years, per gram of waste" (p. 38084, Ref. 2). Specifically, the normalized release R for transuranic waste is defined by

$$R = \sum_i \left(\frac{Q_i}{L_i}\right)\left(1 \times 10^6 \text{ Ci} / C\right), \tag{1}$$

where Q_i is the cumulative release of radionuclide i to the accessible environment during the 10,000-yr period following closure of the repository (Ci), L_i is the release limit for radionuclide i given in Table 1 (Ci) and C is the amount of transuranic waste emplaced in the repository (Ci). In the 1996 WIPP PA, $C = 3.44 \times 10^6$ Ci (Refs. 30, 31). Further, accessible environment means (1) the atmosphere, (2) land surfaces, (3) surface waters, (4) oceans, and (5) all of the lithosphere that is beyond the controlled area; and controlled area means (1) a surface location, to be identified by passive institutional controls, that encompasses no more than 100 square kilometers and extends horizontally no more than five kilometers in any direction from the outer boundary of the original location of the radioactive wastes in a disposal system and (3) the subsurface underlying such a surface location.

To help clarify the intent of 40 CFR 191, the EPA also published 40 CFR 194, *Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with 40 CFR Part 191 Disposal Regulations; Final Rule* (Ref. 32). There, the following elaboration on the intent of 40 CFR 191.13 is given (pp. 5242-5243, Ref. 32):

> § 194.34 Results of performance assessments.
>
> (a) The results of performance assessments shall be assembled into "complementary, cumulative distributions functions" (CCDFs) that represent the probability of exceeding various levels of cumulative release caused by all signficant processes and events.
>
> (b) Probability distributions for uncertain disposal system parameter values used in performance assessments shall be developed and documented in any compliance application.
>
> (c) Computational techniques, which draw random samples from across the entire range of the probability distributions developed pursuant to paragraph (b) of this section, shall be used in generating CCDFs and shall be documented in any compliance application.
>
> (d) The number of CCDFs generated shall be large enough such that, at cumulative releases of 1 and 10, the maximum CCDF generated exceeds the 99th percentile of the population of CCDFs with at least a 0.95 probability.
>
> (e) Any compliance application shall display the full range of CCDFs generated.
>
> (f) Any compliance application shall provide information which demonstrates that there is at least a 95 percent level of statistical confidence that the mean of the population of CCDFs meets the containment requirements of § 191.13 of this chapter.

When viewed at a high level, three basic entities (EN1, EN2, EN3) underlie the results required in 191.13 and 194.34 and ultimately determine the conceptual and computational structure of the 1996 WIPP PA:

EN1, a probabilistic characterization of the likelihood of different futures occurring at the WIPP site over the next 10,000 yr,

EN2, a procedure for estimating the radionuclide releases to the accessible environment associated with each of the possible futures that could occur at the WIPP site over the next 10,000 yr,

EN3, a probabilistic characterization of the uncertainty in the parameters used in the definition of EN1 and EN2.

Together, EN1 and EN2 give rise to the CCDF specified in 191.13(a) (Fig. 1), and EN3 corresponds to the distributions indicated in 194.34(b).

The preceding entities arise from an attempt to answer three questions about the WIPP, Q1: What occurrences could take place at the WIPP site over the next 10,000 yr?

Q2: How likely are the different occurrences that could take place at the WIPP site over the next 10,000 yr?

Q3: What are the consequences of the different occurrences that could take place at the WIPP site over the next 10,000 yr?

and one question about the WIPP PA,

Q4: How much confidence should be placed in answers to the first three questions?

In the 1996 WIPP PA, EN1 provides answers to Q1 and Q2, EN2 provides an answer to Q3, and EN3 provides an answer to Q4. The nature of EN1, EN2 and EN3 and the role that they play in the 1996 WIPP PA are elaborated on in the next three sections.

3. EN1: Probabilistic Characterization of Different Futures (Adapted from Sect. 4, Ref. 26)

The entity EN1 is the outcome of the scenario development process for the WIPP[34] and provides a probabilistic characterization of the likelihood of different futures that could occur at the WIPP site over the next 10,000 yr, with the period of 10,000 yr specified in 40 CFR 191. When viewed formally, EN1 is defined by a probability space ($\mathcal{S}_{st}$, $\mathcal{S}_{st}$, p_{st}), with the sample space $\mathcal{S}_{st}$ given by

$$S_{st} = \{\mathbf{x}_{st} : \mathbf{x}_{st} \text{ is a possible 10,000 yr sequence of occurrences at the WIPP}\}. \quad (2)$$

The subscript *st* refers to stochastic (i.e., aleatory) uncertainty and is used because (S_{st}, $\mathcal{S}_{st}$, p_{st}) is providing a probabilistic characterization of occurrences that may take place in the future.[35]

As a reminder, a probability space (S, $\mathcal{S}$, p) consists of three components: a set S that contains everything that could occur in the particular "universe" under consideration, a suitably restricted set $\mathcal{S}$ of subsets of S, and a function *p* defined for elements of $\mathcal{S}$ that actually defines probability (Sect. IV.4, Ref. 36). In the terminology of probability theory, S is the sample space, the elements of S are elementary events, the subsets of S contained in $\mathcal{S}$ are events, and *p* is a probability measure. In most applied problems, the function *p* defined on $\mathcal{S}$ is replaced by a probability density function (PDF) *d*.

The scenario 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. 1; Ref. 34). In addition, 40 CFR 194 specifies that the occurrence of mining within the land withdrawal boundary must be included in the analysis. As a result, the elements $\mathbf{x}_{st}$ of S_{st} are vectors of the form

$$\mathbf{x}_{st} = [\underbrace{t_1, l_1, e_1, b_1, p_1, \mathbf{a}_1}_{1^{\text{st}}\text{ intrusion}}, \underbrace{t_2, l_2, e_2, b_2, p_2, \mathbf{a}_2}_{2^{\text{nd}}\text{ intrusion}}, \ldots, \underbrace{t_n, l_n, e_n, b_n, p_n, \mathbf{a}_n}_{n^{\text{th}}\text{ intrusion}}, t_{min}] \tag{3}$$

in the 1996 WIPP PA, where n is the number of drilling intrusions, 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 where 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 within the land withdrawal boundary. In the development of $(S_{st}, \mathcal{S}_{st}, p_{st})$, 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 (i.e., the Delaware Basin) in which the WIPP is located. A vector notation is used for $\mathbf{a}_i$ because it is possible for a given drilling intrusion to penetrate several different types of waste. Further, the probabilistic characterization for t_{min} follows from the guidance in 40 CFR 194 that the occurrence of potash mining within the land withdrawal boundary should be assumed to occur randomly in time (i.e., follow a Poisson process with a rate constant of $\lambda_m = 10^{-4}\ \text{yr}^{-1}$), with all commercially viable potash reserves within the land withdrawal boundary being extracted at time t_{min}.

With respect to the previously indicated questions, S_{st} provides an answer to Q1, while $\mathcal{S}_{st}$ and p_{st} provide an answer to Q2. In practice, Q2 will be answered by specifying distributions for n, t_i, l_i, e_i, b_i, p_i, $\mathbf{a}_i$, and t_{min}, which in turn lead to definitions for $\mathcal{S}_{st}$ and p_{st}. The CCDF in 40 CFR 191 will be obtained by evaluating an integral involving $(S_{st}, \mathcal{S}_{st}, p_{st})$ (Fig. 2). The definition of $(S_{st}, \mathcal{S}_{st}, p_{st})$ is discussed in more detail in Ref. 37.

4. EN2: Estimation of Releases (Adapted from Sect. 5, Ref. 26)

The entity EN2 is the outcome of the model development process for the WIPP and provides a procedure for estimating radionuclide releases to the accessible environment for the different futures (i.e., elements $\mathbf{x}_{st}$ of S_{st}) that could occur at the WIPP. Insights on the processes to be modeled were provided as part of the scenario development process.[34]

This procedure can be represented by a function $f(\mathbf{x}_{st})$. In practice, f is quite complex and is based on the models implemented in the computer programs indicated in Fig. 3 and Table 2. In the context of these models, f has the form

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

$$+ f_{MB}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right] + f_{DL}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right] + f_{S}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$$

$$+ f_{S-T}\left\{\mathbf{x}_{st,0}, f_{S-F}\left(\mathbf{x}_{st,0}\right), f_{N-P}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]\right\} \tag{4}$$

in the 1996 WIPP PA, 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 for $\mathbf{x}_{st}$ calculated with CUTTINGS_S,

$f_B(\mathbf{x}_{st})$ ~ two-phase flow results calculated for $\mathbf{x}_{st}$ with BRAGFLO; in practice, $f_B(\mathbf{x}_{st})$ is a vector containing a large amount of information,

$f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ spallings release to accessible environment for $\mathbf{x}_{st}$ calculated with the spallings model contained in CUTTINGS_S; this calculation requires BRAGFLO results (i.e., $f_B(\mathbf{x}_{st})$) as input,

$f_{DBR}\{\mathbf{x}_{st}, f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})], f_B(\mathbf{x}_{st})\}$ ~ direct brine release to accessible environment for $\mathbf{x}_{st}$ calculated with a modified version of BRAGFLO designated BRAGFLO_DBR; this calculation requires spallings results obtained from CUTTINGS_S (i.e., $f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$) and BRAGFLO results (i.e., $f_B(\mathbf{x}_{st})$) as input,

$f_{MB}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release through anhydrite marker beds to accessible environment for $\mathbf{x}_{st}$ calculated with NUTS; this calculation requires BRAGFLO results (i.e., $f_B(\mathbf{x}_{st})$) as input,

$f_{DL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release through Dewey Lake Red Beds to accessible environment for $\mathbf{x}_{st}$ calculated with NUTS; this calculation requires BRAGFLO results (i.e., $f_B(\mathbf{x}_{st})$) as input,

$f_S[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release to land surface due to brine flow up a plugged borehole for $\mathbf{x}_{st}$ calculated with NUTS or PANEL; this calculation requires BRAGFLO results (i.e., $f_B(\mathbf{x}_{st})$) as input,

$f_{S-F}(\mathbf{x}_{st,0})$ ~ flow field calculated for $\mathbf{x}_{st,0}$ with SECOFL2D,

$f_{N-P}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release to Culebra for $\mathbf{x}_{st}$ calculated with NUTS or PANEL as appropriate; this calculation requires BRAGFLO results (i.e., $f_B(\mathbf{x}_{st})$) as input,

$f_{S-T}\left\{\mathbf{x}_{st,0}, f_{S-F}\left(\mathbf{x}_{st,0}\right), f_{N-P}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]\right\}$ ~ groundwater transport release through Culebra to accessible environment calculated with SECOTP2D; this calculation requires SECOFL2D results (i.e., $f_{S-F}(\mathbf{x}_{st,0})$) and NUTS or PANEL results (i.e., $f_{N-P}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$) as input; $\mathbf{x}_{st,0}$ is used as an argument to f_{S-T} because drilling intrusions are assumed to cause no perturbations to the flow field in the Culebra.

The probability space $(\mathcal{S}_{st}, \mathscr{S}_{st}, p_{st})$ and the function f give rise to the CCDF specified in 40 CFR 191.13(a), which can be represented as integral of f over $\mathcal{S}_{st}$ (Fig. 2). The models that underlie f (Fig. 3, Table 2) are too complex to permit a closed form evaluation of the integral in Fig. 2 that defines the CCDF specified in 40 CFR 191. Rather, a Monte Carlo procedure is used in the 1996 WIPP PA. Specifically, elements

$$\mathbf{x}_{st,i},\ i = 1, 2, \ldots, nS, \tag{5}$$

are randomly sampled from $\mathcal{S}_{st}$ in consistency with the definition of $(\mathcal{S}_{st}, \mathscr{S}_{st}, p_{st})$. Then, the integral in Fig. 2, and hence the associated CCDF, is approximated by

$$prob(Rel > R) = \int_{\mathcal{S}_{st}} \delta_R\left[f\left(\mathbf{x}_{st}\right)\right] d_{st}\left(\mathbf{x}_{st}\right) dV_{st} \doteq \sum_{i=1}^{nS} \delta_R\left[f\left(\mathbf{x}_{st,i}\right)\right] / nS, \tag{6}$$

where $\delta_R[f(\mathbf{x}_{st})] = 1$ if $f(\mathbf{x}_{st}) > R$ and 0 if $f(\mathbf{x}_{st}) \leq R$ and d_{st} is the density function associated with the probability space $(\mathcal{S}_{st}, \mathscr{S}_{st}, p_{st})$ for stochastic uncertainty.[54] The manner in which the random sampling from $\mathcal{S}_{st}$ and associated CCDF construction is carried out is described in Ref. 37.

The models that underlie f are too computationally intensive to permit their evaluation for every element $\mathbf{x}_{st,i}$ of $\mathcal{S}_{st}$ in Eq. (5). Due to this constraint, these models are evaluated for representative elements of $\mathcal{S}_{st}$, and then the results of these evaluations are used to construct values of f for the large number of $\mathbf{x}_{st,i}$ (i.e., $nS = 10{,}000$ in the 1996 WIPP PA) in Eq. (5). The specific elements of $\mathcal{S}_{st}$ for which calculations are performed are described in Sect. 12 of Ref. 37, and the associated construction procedures for other elements of $\mathcal{S}_{st}$ are described in Ref. 44 for f_C and f_{SP}, Ref. 41 for f_{DBF}, Ref. 48 for f_{MB}, f_{DL}, f_S and f_{N-P}, and Ref. 53 for f_{S-T}.

With respect to the previously indicated questions, the models that underlie the function f in Eq. (4) are providing an answer to Q3. These models, and hence the function f, are discussed in more detail in Refs. 39, 41, 44, 48, 53.

5. EN3: Probabilistic Characterization of Parameter Uncertainty (Adapted from Sect. 6, Ref. 26)

The entity EN3 is the outcome of the data development effort for the WIPP and provides a probabilistic characterization of the uncertainty in the parameters that underlie the WIPP PA. When viewed formally, EN3 is defined by a probability space $(\mathrm{S}_{su}, \mathcal{S}_{su}, p_{su})$, with the sample space S_{su} given by

$$\mathrm{S}_{su} = \{\mathbf{x}_{su}\text{: } \mathbf{x}_{su} \text{ is possibly the correct vector of parameter values to use in the WIPP PA models}\}. \tag{7}$$

The subscript *su* refers to subjective (i.e., epistemic) uncertainty and is used because $(\mathrm{S}_{su}, \mathcal{S}_{su}, p_{su})$ is providing a probabilistic characterization of where the appropriate inputs to use in the WIPP PA are believed to be located.[35] In practice, some elements of $\mathbf{x}_{su}$ could affect the definition of $(\mathrm{S}_{st}, \mathcal{S}_{st}, p_{st})$ (e.g., the rate constant λ used to define the Poisson process for drilling intrusions or the probability that a randomly placed drilling intrusion will penetrate pressurized brine in the Castile Fm) and other elements could relate to the models in Fig. 3 and Table 2 that determine the function f in Eq. (4) and Fig. 3 (e.g., radionuclide solubilities in Castile brine or fracture spacing in the Culebra Dolomite). However, in the 1996 WIPP PA, all elements of $\mathbf{x}_{su}$ relate to the models in Fig. 3 and Table 2.

If the value for $\mathbf{x}_{su}$ was precisely known, then the CCDF in Fig. 2 could be determined with certainty and compared with the boundary line specified in 40 CFR 191. However, given the complexity of the WIPP site and the 10,000 yr time period under consideration, $\mathbf{x}_{su}$ can never be known with certainty. Rather, uncertainty in $\mathbf{x}_{su}$ as characterized by $(\mathrm{S}_{su}, \mathcal{S}_{su}, p_{su})$ will lead to a distribution of CCDFs (Fig. 4), with a different CCDF resulting for each possible value that $\mathbf{x}_{su}$ can take on. The proximity of this distribution to the boundary line in Fig. 2 provides an indication of the confidence with which 40 CFR 191 will be met.

The distribution of CCDFs in Fig. 4 can be summarized by distributions of exceedance probabilities conditional on individual release values (Fig. 5). For a given release value R, this distribution is defined by a double integral over S_{su} and S_{st} (Refs. 33, 35). In practice, this integral is too complex to permit a closed-form evaluation. Instead, the WIPP PA uses Latin hypercube sampling[55] to evaluate the integral over S_{su} and, as indicated in Eq. (6), simple random sampling to evaluate the integral over S_{st}. Specifically, a Latin hypercube sample (LHS)

$$\mathbf{x}_{su,k},\ k = 1, 2, \ldots, nLHS, \tag{8}$$

is generated from S_{su} in consistency with the definition of $(\mathrm{S}_{su}, \mathcal{S}_{su}, p_{su})$ and a random sample $\mathbf{x}_{st,i}$, $i = 1, 2, \ldots, nS$, as indicated in Eq. (5) is generated from S_{st} in consistency with the definition of $(\mathrm{S}_{st}, \mathcal{S}_{st}, p_{st})$. The probability $prob(p \le P|R)$ in Fig. 5 is then approximated by

$$prob(p \le P|R) \doteq 1 - \sum_{k=1}^{nLHS} \delta_P\left[\sum_{i=1}^{nS} \delta_R\left[f\left(\mathbf{x}_{st,i}, \mathbf{x}_{su,k}\right)\right] / nS\right] / nLHS, \tag{9}$$

where $prob(p \le P|R)$ designates the probability that the exceedance probability (i.e., p) for a release of size R will be less than or equal to P, and δ_R, and also δ_P, are defined the same as δ_R in Eq. (6). The result of the preceding calculation is typically displayed by plotting percentile values (e.g., $P_{0.1}$, $P_{0.5}$, and $P_{0.9}$ from Fig. 5), which are obtained by solving Eq. (9) for P with $prob(p \le P|R) = 0.1$, 0.5 and 0.9, respectively, and also mean values (i.e., $\overline{P}$ from Fig. 5) for exceedance probabilities above the corresponding release values (i.e., R) and then connecting these points to form continuous curves (Fig. 6). The proximity of these curves to the indicated boundary line provides an indication of the confidence with which 40 CFR 191 will be met.

With respect to the previously indicated questions, $(\mathcal{S}_{su}, \mathcal{S}_{su}, p_{su})$ and results derived from $(\mathcal{S}_{su}, \mathcal{S}_{su}, p_{su})$ (e.g., the distributions in Figs. 4 - 6) are providing an answer to Q4. The definition of $(\mathcal{S}_{su}, \mathcal{S}_{su}, p_{su})$ and the generation of the Latin hypercube sample in Eq. (7) are discussed in Ref. 56.

Generation of the LHS in Eq. (8) and evaluation of the function f in Eq. (4) for selected elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$ (see Sect. 12, Ref. 37) generates a mapping

$$[\mathbf{x}_{su,k}, f(\mathbf{x}_{st}, \mathbf{x}_{su,k})],\ k = 1, 2, \ldots, nLHS, \tag{10}$$

from uncertain analysis inputs to analysis results. More generally, the mapping can be expressed as

$$[\mathbf{x}_{su,k}, \mathbf{y}(\mathbf{x}_{su,k})],\ k = 1, 2, \ldots, nLHS, \tag{11}$$

where $\mathbf{y}(\mathbf{x}_{su,k})$ denotes the results obtained with the model or models under consideration. A vector rotation is used for $\mathbf{y}$ because, in general, a large number of predicted results is produced by each of the models used in the 1996 WIPP PA; in addition, $\mathbf{y}(\mathbf{x}_{su,k})$ could also correspond to a CCDF constructed from model results associated with $\mathbf{x}_{su,k}$.

Once generated, the mappings in Eqs. (10) and (11) provide a summary of the (subjective) uncertainty in f and $\mathbf{y}$, and can be explored with sensitivity analysis techniques based on the examination of scatterplots, regression analysis and correlation analysis (Sect. 9, Ref. 56; Sect. 3.5, Ref. 57). Uncertainty and sensitivity analysis results for individual components of f (i.e., $f_B, f_C, f_{SP}, f_{DBR}, f_{MB}, f_{DL}, f_S, f_{N-P}, f_{S-T}$) are given in Refs. 41, 44, 48, 53, 59, 60. Further, uncertainty and sensitivity analysis results for CCDFs are given in Refs. 41, 44, 48, 53, 60.

6. Historical Perspective (Adapted from Ref. 61)

The importance of identifying, characterizing and displaying the uncertainty in the outcomes of analyses for complex systems is now widely recognized. The EPA's requirements for such results are explicitly stated in the quotes from 40 CFR 191 and 40 CFR 194 in Sect. 2. As other examples, the following statements are made in the indicated documents:

Risk Assessment in the Federal Government: Managing the Process (p. 148, Ref. 62)

> Preparation of fully documented written risk assessments that explicitly define the judgments made and attendant uncertainties clarifies the agency decision-making process and aids the review process considerably.

Safety Goals for the Operation of Nuclear Power Plants (p. 30031, Ref. 63)

> The Commission is aware that uncertainties are not caused by use of quantitative methodology in decisionmaking but are merely highlighted through use of the quantification process. Confidence in the use of probabilistic and risk assessment techniques has steadily improved since the time these were used in the Reactor Safety Study. In fact, through use of quantitative techniques, important uncertainties have been and continue to be brought into better focus and may even be reduced compared to those that would remain with sole reliance on deterministic decisionmaking. To the extent practicable, the Commission intends to ensure that the quantitative techniques used for regulatory decisionmaking take into account the potential uncertainties that exist so than an estimate can be made on the confidence level to be ascribed to the quantitative results.

Issues in Risk Assessment (p. 329, Ref. 64)

- *A discussion of uncertainty should be included in any ecological risk assessment.* Uncertainties could be discussed in the methods section of a report, and the consequences of uncertainties described in the discussion section. End-point selection is an important component of ecological risk assessment. Uncertainties about the selection of end points need to be addressed.

- *Where possible, sensitivity analysis, Monte Carlo parameter uncertainty analysis, or another approach to quantifying uncertainty should be used.* Reducible uncertainties (related to ignorance and sample size) and irreducible (aleatory) uncertainties should be clearly distinguished. Quantitative risk estimates, if presented, should be expressed in terms of distributions rather than as point estimates (especially worst-case scenarios).

An SAB Report: Multi-Media Risk Assessment for Radon, Review of Uncertainty Analysis of Risks Associated with Exposure to Radon (pp. 24–25, Ref. 65)

> The Committee believes strongly that the explicit disclosure of uncertainty in quantitative risk assessment is necessary any time the assessment is taken beyond a screening calculation. ...
>
> The need for regulatory action must be based on more realistic estimates of risk. Realistic risk estimating, however, requires a full disclosure of uncertainty. The disclosure of uncertainty enables the scientific reviewer, as well as the decision-maker, to evaluate the degree of confidence that one should have in the risk assessment. The confidence in the risk assessment should be a major factor in determining strategies for regulatory action.
>
> Large uncertainty in the risk estimate, although undesirable, may not be critical if the confidence intervals about the risk estimate indicate that risks are clearly below regulatory levels of concern. On the other hand, when these confidence intervals overlap the regulatory levels of concern, consideration should be given to acquiring additional information to reduce the uncertainty in the

> risk estimate by focusing research on the factors that dominate the uncertainty. The dominant factors controlling the overall uncertainty are readily identified through a sensitivity analysis conducted as an integral part of quantitative uncertainty analysis. Acquiring additional data to reduce the uncertainty in the risk estimates is especially important when the cost of regulation is high. Ultimately, the explicit disclosure (of the uncertainty) in the risk estimate should be factored into analyses of the cost-effectiveness of risk reduction as well as in setting priorities for the allocation of regulatory resources for reducing risk.

Science and Judgment in Risk Assessment[66]

> A distinction between uncertainty (i.e., degree of potential error) and inter-individual variability (i.e., population heterogeneity) is generally required if the resulting quantitative risk characterization is to be optimally useful for regulatory purposes, particularly insofar as risk characterizations are treated quantitatively.
>
> - The distinction between uncertainty and individual variability ought to be maintained rigorously at the level of separate risk-assessment components (e.g., ambient concentration, uptake and potency) as well as at the level of an integrated risk characterization. (p. 242)
>
> When reporting estimates of risk to decision-makers and the public, EPA should report not only point estimates of risk but also the sources and magnitudes of uncertainty associated with these estimates. (p. 263)
>
> Because EPA often fails to characterize fully the uncertainty in risk assessments, inappropriate decisions and insufficiently or excessively conservative analyses can result. (p. 267)

Guiding Principles for Monte Carlo Analysis (p. 3, Ref. 67)

> ... the basic goal of a Monte Carlo analysis is to characterize, quantitatively, the uncertainty and variability in estimates of exposure or risk. A secondary goal is to identify key sources to the overall variance and range of model results.
>
> Consistent with EPA principles and policies, an analysis of variability and uncertainty should provide its audience with clear and concise information on the variability in individual exposures and risks; it should provide information on population risk (extent of harm in the exposed population); it should provide information on the distribution of exposures and risks to highly exposed or highly susceptible populations; it should describe qualitatively and quantitatively the scientific uncertainty in the models applied, the data utilized, and the specific risk estimates that are used.

When viewed at a high level, the uncertainty referred to in 40 CFR 191, 194 (Sect. 2) and also in the preceding quotes can usually be divided into two types: stochastic (i.e., aleatory) uncertainty, which arises because the system under study can behave in many different ways and is thus a property of the system, and subjective (i.e., epistemic) uncertainty, which arises from a lack of knowledge about the system and is thus a property of the analysts performing the study. When a distinction between stochastic and subjective uncertainty is not maintained, the deleterious events associated with a system, the likelihood of such events, and the confidence with which both likelihood and consequences can be estimated become commingled in a way that makes it difficult to draw useful insights. Due to the pervasiveness and importance of these two types of uncertainty, they have attracted many investigators (e.g., Refs. 20, 35, 68 - 87) and also many names (e.g., 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). Indeed, this distinction can be traced back to the beginnings of the formal development of probability theory in the seventeenth century.[88, 89]

As an example, probabilistic risk assessments (PRAs) for nuclear power plants and other complex engineered facilities involve stochastic uncertainty due to the many different types of accidents that can occur and subjective uncertainty due to the inability of the analysts involved to precisely determine the frequency and consequences of these accidents. The recent reassessment of the risk from nuclear power plants conducted by the U.S. Nuclear Regulatory Commission (NUREG-1150) provides an example of a very large analysis in which an extensive effort was made to separate stochastic and subjective uncertainty (Refs. 80, 90). This analysis was instituted in response to criticisms that the Reactor Safety Study[91] had inadequately characterized the uncertainty in its results.[92] Similarly, the EPA's standard for the geologic disposal of radioactive waste (Sect. 2) can be interpreted as requiring (1) the estimation of a CCDF, which arises from the different disruptions that could occur at a waste disposal site and is thus a summary of the effects of stochastic uncertainty (Sect. 3), and (2) the assessment of the uncertainty associated with the estimation of this CCDF, with this uncertainty deriving from a lack of knowledge on the part of the analysts involved and thus providing a representation for the effects of subjective uncertainty (Sect. 5). Conceptually, similar problems also arise in the assessment of health effects within a population exposed to a carcinogenic chemical or some other stress, where variability within the population can be viewed as stochastic uncertainty and the inability to exactly characterize this variability and estimate associated exposures and health effects can be viewed as subjective uncertainty (e.g., Refs. 93 - 99). Other examples also exist of analyses that maintain a separation of stochastic and aleatory uncertainty (e.g., Refs. 100 - 104). Thus, by maintaining a separation between stochastic and subjective uncertainty as indicated in Sects. 3-5 and described in more detail in other articles (Refs. 37, 41, 44, 48, 53, 56, 60), the 1996 WIPP Pa is in the main stream of current analyses for complex systems.

Many individuals believe that the boundary line associated with 40 CFR 191.13 and illustrated in Fig. 1 is a novel concept. Actually, this construction is an example of the Farmer limit line approach to the definition of acceptable risk.[105-107] A similar construction was used in the NUREG-1150 analyses[80, 90] to implement the proposed large release safety goal for reactor accidents.[63, 108] Thus, again, the 1996 WIPP PA involves widely used ideas, although the actual scale of the analysis is much larger than that of a typical PA.

7. Discussion

This article presents a formal description of the conceptual structure of the 1996 WIPP PA. In particular, the structure of the PA is described in terms of a probability space $(S_{st}, \mathcal{S}_{st}, p_{st})$ for stochastic (i.e., aleatory) uncertainty, a probability space $(S_{su}, \mathcal{S}_{su}, p_{su})$ for subjective (i.e., epistemic) uncertainty, and a function $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ defined for elements $\mathbf{x}_{st}$ and $\mathbf{x}_{su}$ of the sample spaces S_{st} and S_{su}. The probability space $(S_{st}, \mathcal{S}_{st}, p_{st})$ characterizes the likelihood of different 10,000 yr futures (i.e., $\mathbf{x}_{st}$) that could occur at the WIPP and underlies the CCDF specified by the EPA in 40 CFR 191; the probability space $(S_{su}, \mathcal{S}_{su}, p_{su})$ characterizes a degree of belief with respect to where the appropriate parameter values for use in the 1996 WIPP PA (i.e., $\mathbf{x}_{su}$) are located; and the function $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ estimates normalized radionuclide releases (and, in general, many other quantities) that derive from $\mathbf{x}_{st}$ and $\mathbf{x}_{su}$.

Introduction of this formal description of the structure of the 1996 WIPP PA provides a way to give names and symbols to the important parts of the analysis. Once names and symbols are assigned, it is then possible to unambiguously describe the individual parts of the PA and how these parts fit together to make the complete PA. Without these names and symbols, it is difficult to give a precise description of the individual parts of the PA and how these parts come together in the computational implementation of the PA.

As an example, large PAs make extensive and sometimes complex use of probability. In such applications, it is essential to understand how probability is being used, and in particular, to what type of "entity" probability is being assigned. As a start, it is essential to know what the sample space is. It is always disconcerting to realize that a probabilistic calculation is being carried out without a clear concept of what the sample space is. In the 1996 WIPP PA, there are two distinct sample spaces (i.e., S_{st} and S_{su}), each with its elements (i.e., $\mathbf{x}_{st}$ and $\mathbf{x}_{su}$) clearly defined. A suggestion: When considering a probabilistic calculation, always ask yourself, or the individuals carrying out the calculation, what constitutes the sample space. Without a satisfactory answer to this question, a clear understanding of the calculation cannot be developed.

The use of a formal structure to describe the 1996 WIPP PA provides a way to distinguish between concept and approximation. For example, the 1996 WIPP PA presents uncertainty distributions arising from stochastic uncertainty alone, subjective uncertainty alone, and stochastic and subjective uncertainty combined. Such distributions can be unambiguously defined in terms of integrals over S_{st} and/or S_{su}. Such integrals provide a way to express exactly what is being calculated but do not constitute a suitable computational procedure; rather, they must be approximated with some type of numerical procedure. The 1996 WIPP PA used simple random sampling for integrations involving the probability space $(S_{st}, \mathcal{S}_{st}, p_{st})$ and Latin hypercube sampling for integrations involving the probability space $(S_{su}, \mathcal{S}_{su}, p_{su})$. The use of such sampling-based numerical approximations is often referred to as Monte Carlo analysis.

As an aside, some individuals express concern, or worse, over the use of Monte Carlo analyses. Given that Monte Carlo analysis is just a way to approximate an integral, this does not really make sense (would the same concern be expressed if the analysts stated that a Gaussian quadrature procedure was being used to evaluate the integral in question?) Rather, if there is reason for concern, it should be respect to the appropriateness of the function being integrated or the probability space being integrated over. The particular integration procedure being used should not be an object of concern beyond considerations of convergence and accuracy.

A benefit of representing a PA with probability spaces, functions and integrals is that it provides a description of the PA in the same notation that is used in formal developments of probability. This representation of the PA in a widely used format facilitates understanding of the conceptual and computational details of the PA within the PA project itself and the communication of these details to reviewers and other individuals outside the project. For example, such a representation helps clarify the concept of a scenario, with a scenario being either a subset E_{st} of the sample space S_{st} for stochastic uncertainty (i.e., an element of $\mathcal{S}_{st}$), a subset E_{su} of the sample space S_{su} for subjective uncertainty (i.e., and element of $\mathcal{S}_{su}$) or a subset E of $S = S_{st} \times S_{su}$ (i.e., an element of $\mathcal{S}_{st} \times \mathcal{S}_{su}$). Thus, a scenario is what is typically called an event in a formal development of probability and the corresponding scenario probabilities are given by $p_{st}(E_{st})$, $p_{su}(E_{su})$ and $p(E) = p_{st}(E_{st})\ p_{su}(E_{su})$, respectively, where the representation for the probability of E (i.e., $p(E)$) holds provided $E = E_{st} \times E_{su}$ and the elements of E_{st} and E_{su} are independent in a probabilistic sense (i.e., the occurrence of E_{st} has no effect on the occurrence of E_{su} and vice versa). The preceding indicates three distinct, but legitimate, uses of the concept of a scenario. Because these three uses involve different types of occurrences, it is important to clearly indicate which usage is intended when the idea of a scenario is employed. A careful definition of the underlying probability spaces provides a basis for such an indication.

A formal use of probability also helps clarify what types of events (i.e., scenarios) can have nonzero probabilities. For example, it is important to recognize that individual elements of S_{st} (i.e., 10,000 yr futures at the WIPP) or S_{su} (e.g., elements of the LHS used to propagate subjective uncertainty) have a probability of zero. The single exception is the element $\mathbf{x}_{st}$ of S_{st} corresponding to undisturbed conditions. Thus, with this one exception, nonzero probabilities only apply to subsets of S_{st}, S_{su} and $S_{st} \times S_{su}$ containing infinitely many elements. This is an important conceptual point that affects how results are interpreted. In random and LHS procedures, individual sample elements are assigned a weight equal to the reciprocal of the sample size (i.e., $1/nS$, $1/nLHS$) for use in estimating expected values and distributions; however, such weights are not the same as probabilities.

The formal representation also helps show how different analysis approaches are simply different ways of approximating the same quantities. For example, the Kaplan/Garrick ordered triple representation for risk[68] might initially appear to be quite different from the sampling-based approach used in the 1996 WIPP PA. However, the Kaplan/Garrick approach and the sampling-based approach used in the 1996 WIPP PA are simply different ways of approximating integrals involving the probability spaces $(S_{st}, \mathcal{S}_{st}, p_{st})$ and $(S_{su}, \mathcal{S}_{su}, p_{su})$. A proper level of abstraction makes this easily apparent (Sect. 13, Ref. 37). Further, modern probabilistic risk assessments (PRAs) for nuclear power stations have exactly the same conceptual structure as the 1996 WIPP PA, although the processes under consideration and the models in use are very different. Again, a description of these analyses at an appropriate level of abstraction makes this similarity readily apparent.[35, 82]

Now that the overall structure of the 1996 WIPP PA has been summarized in terms of a probability space (S_{st}, $\mathcal{S}_{st}$, p_{st}) for stochastic uncertainty, a probability space (S_{su}, $\mathcal{S}_{su}$, p_{su}) for subjective uncertainty and a function f defined on $S_{st} \times S_{su}$, detailed information on (S_{st}, $\mathcal{S}_{st}$, p_{st}), (S_{st}, $\mathcal{S}_{st}$, p_{st}) and f and their use in the 1996 WIPP PA can be obtained from other articles. In particular, (S_{st}, $\mathcal{S}_{st}$, p_{st}) is described in Ref. 37; (S_{su}, $\mathcal{S}_{su}$, p_{su}) is described in Ref. 56; f and its component functions are described in Refs. 39, 41, 44, 48, 53; the construction of CCDFs for comparison with the release limits specified in 40 CFR 191 is discussed in Refs. 41, 44, 48, 53, 60; and uncertainty and sensitivity analysis for both individual model results (i.e., evaluations of f and its component functions) and CCDFs is discussed in Refs. 41, 44, 48, 53, 58, 59, 60.

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Figure Captions

Fig. 1. Boundary line and associated CCDF specified in 40 CFR 191, Subpart B (Fig. 1, Ref. 33).

Fig. 2. Definition of CCDF specified in 40 CFR 191, Subpart B as an integral involving the probability space ($\mathcal{S}_{st}$, $\mathcal{S}_{st}$, p_{st}) for stochastic uncertainty and a function f defined on S_{st} (Fig. 5, Ref. 25).

Fig. 3. Models used in 1996 WIPP PA (Fig. 4, Ref. 25).

Fig. 4. Distribution of CCDFs resulting from possible values for $\mathbf{x}_{su} \in S_{su}$ (Fig. 6, Ref. 26).

Fig. 5. Distribution of exceedance probabilities due to subjective uncertainty(Fig. 7, Ref. 26).

Fig. 6. Example CCDF distribution from 1992 WIPP PA (Fig. 10, Ref. 12; Fig. 14, Ref. 35).

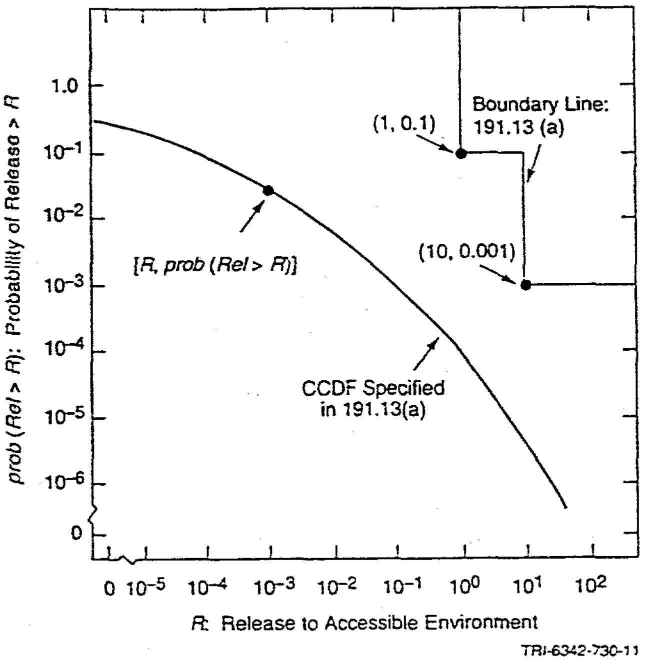

Fig. 1. Boundary line and associated CCDF specified in 40 CFR 191, Subpart B (Fig. 1, Ref. 33).

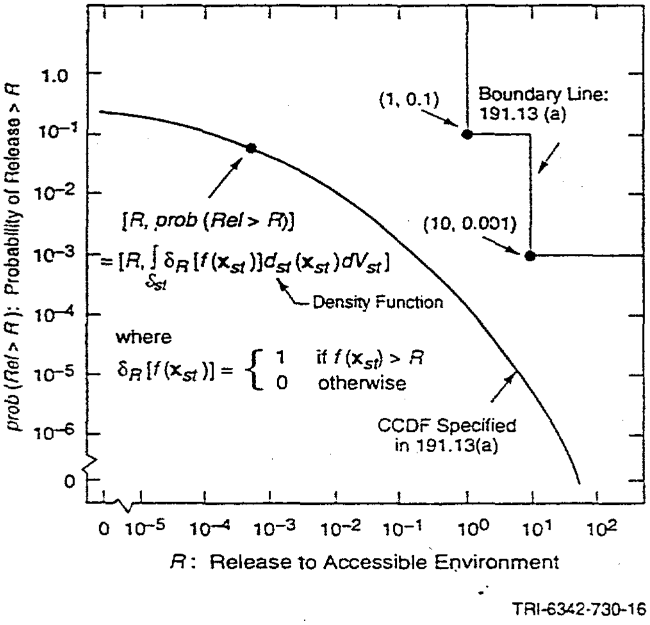

Fig. 2. Models used in 1996 WIPP PA (Fig. 5. Ref. 25).

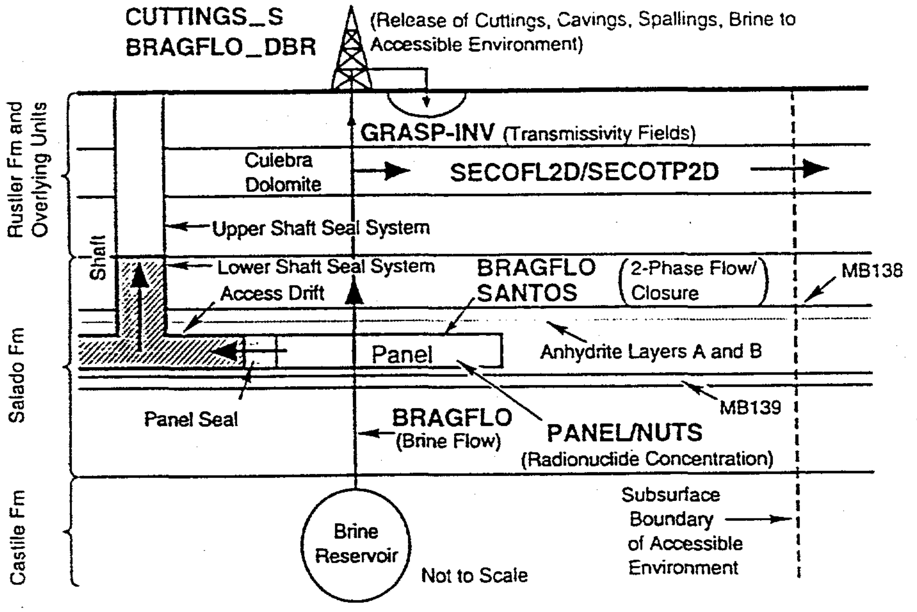

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Fig. 3. Definition of CCDF specified in 40 CFR 191, Subpart B as an integral involving the probability space ($\mathcal{S}_{st}$, $\mathcal{L}_{st}$, p_{st}) for stochastic uncertainty and a function f defined on $\mathcal{S}_{st}$ (Fig. 4, Ref. 25).

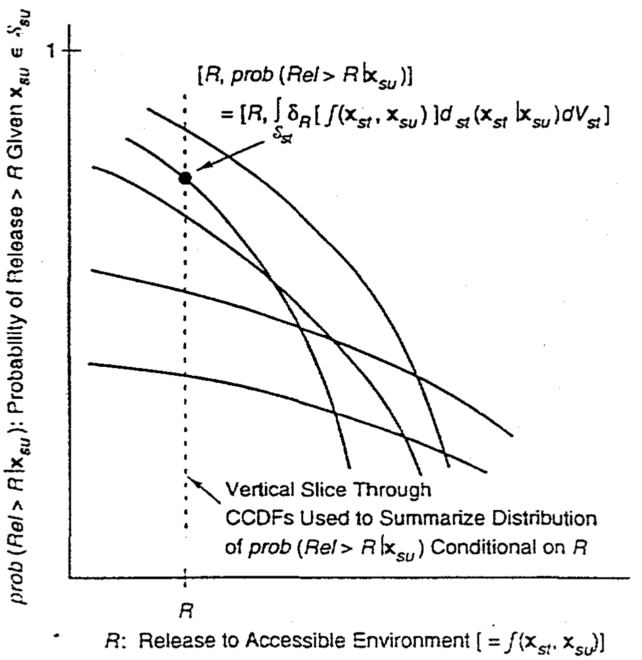

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Fig. 4. Distribution of CCDFs resulting from possible values for $\mathbf{x}_{su} \in \mathcal{S}_{su}$ (Fig. 6, Ref. 26).

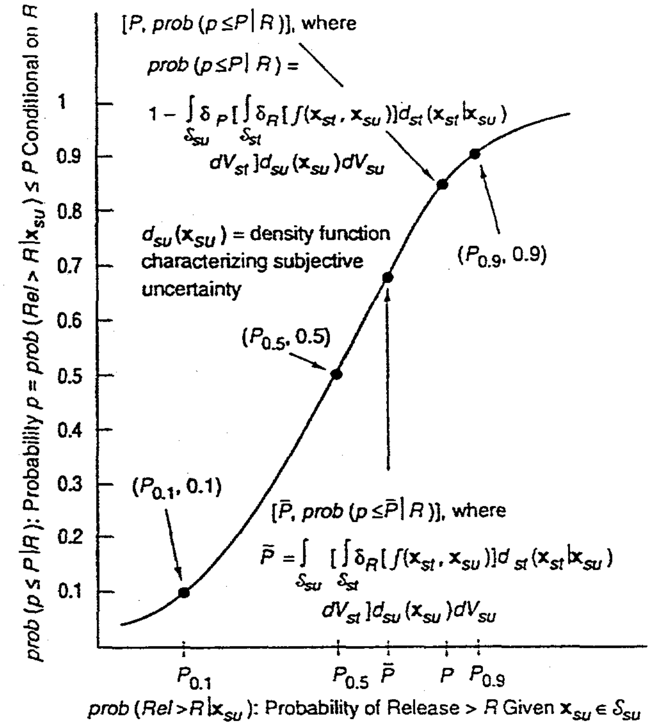

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Fig. 5. Distribution of exceedance probabilities due to subjective uncertainty (Fig. 7, Ref. 26).

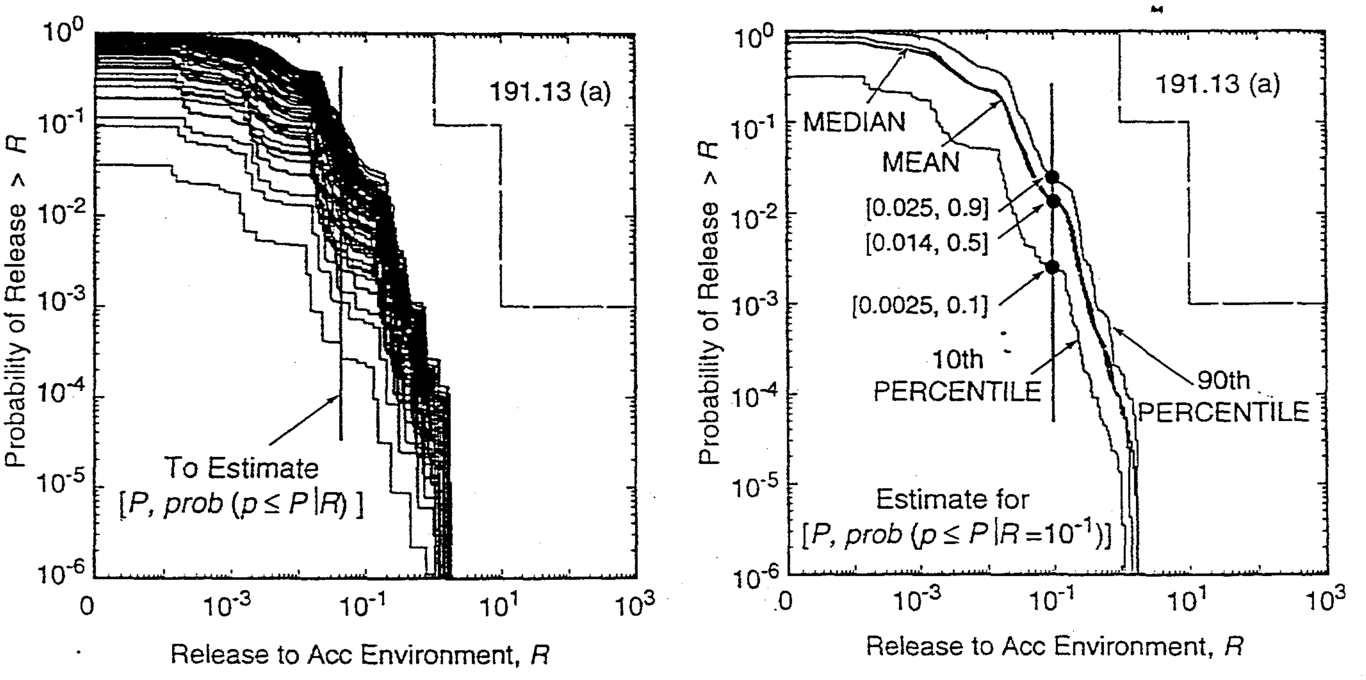

Fig. 6. Example CCDF distribution from 1992 WIPP PA (Fig. 10, Ref. 12; Fig. 14, Ref. 35).

Table 1. Release Limits for the Containment Requirements (Table 1, App. A, Ref. 2)

Radionuclide	Release Limit L_i per 1000 MTHM[a] or other unit of waste[b]
Americium-241 or -243	100
Carbon 14	100
Cesium-135 or -137	1,000
Iodine-129	100
Neptunium-237	100
Plutonium-238, -239, -240, or -242	100
Radium-226	100
Strontium-90	1,000
Technetium-99	10,000
Thorium-230 or -232	10
Tin-126	1,000
Uranium-233, -234, -235, -236, or -238	100
Any other alpha-emitting radionuclide with a half-life greater than 20 yrs	100
Any other radionuclide with a half-life greater than 20 yrs that does not emit alpha particles	1,000

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[a] Metric tons of heavy metal exposed to a burnup between 25,000 megawatt-days per metric ton of heavy metal (MWd/MTHM) and 40,000 MWd/MTHM

[b] An amount of transuranic wastes containing one million curies of alpha-emitting transuranic radionuclides with half-lives greater than 20 yrs

Table 2. Summary of Computer Models Used in the 1996 WIPP PA (Table 1, Ref. 25)

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. Additional information: Ref. 38; Sect. 4.2, Ref. 28; Ref. 39.

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. Additional information: Ref. 40; Sect. 4.7, Ref. 28; Ref. 41.

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. Additional information: Refs. 42, 43; Sects. 4.5, 4.6, Ref. 28; Ref. 44.

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. Additional information: Refs. 45, 46.

NUTS: Solves system of partial differential equations for radionuclide transport in vicinity of repository. Uses brine volumes and flows calculated by BRAGFLO as input. Additional information: Ref. 47; Sect. 4.3, Ref. 28; Ref. 48.

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 solution of system of linear ordinary differential equations. Additional information: Ref. 47; Sect. 4.4, Ref. 28; Ref. 48.

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. Additional information: Ref. 38; Refs. 49, 50; Sect. 4.2.3, Ref. 28.

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. Additional information: Refs. 51, 52; Sect. 4.8, Ref. 28; Ref. 53.

SECOTP2D: Simulates transport of radionuclides in fractured porous media. Solves two partial differential equations: one provides two-dimensional representation for convective and diffusive radionuclide transport in fractures and the other provides one-dimensional representation for diffusion of radionuclides into rock matrix surrounding the fractures. Uses flow fields calculated by SECOFL2D. Additional information: Refs. 51, 52; Sect. 4.9, Ref. 28; Ref. 53.