A Monte Carlo Procedure for the Construction of Complementary Cumulative Distribution Functions for Comparison with the EPA Release Limits for Radioactive Waste Disposal

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ABSTRACT

A Monte Carlo procedure for the construction of complementary cumulative distribution functions (CCDFs) for comparison with the U.S. Environmental Protection Agency (EPA) release limits for radioactive waste disposal (40 CFR 191, Subpart B) is described and illustrated with results from a recent performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The Monte Carlo procedure produces CCDF estimates similar to those obtained with stratified sampling in several recent PAs for the WIPP. The advantages of the Monte Carlo procedure over stratified sampling include increased resolution in the calculation of probabilities for complex scenarios involving drilling intrusions and better use of the necessarily limited number of mechanistic calculations that underlie CCDF construction.

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1. Introduction

The U.S. Environmental Protection Agency (EPA) has promulgated the following containment requirement for the geologic disposal of radioactive waste:^{1,2}

§ 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.

Further, "accessible environment" means (a) the atmosphere, (b) land surfaces, (c) surface waters, (d) oceans, and (e) all of the lithosphere that is beyond the controlled area, and "controlled area" means (a) a surface location, to be identified by passive institutional controls, that encompasses no more than 100 km² and extends horizontally no more than 5 km in any direction from the outer boundary of the original location of the radioactive wastes in a disposal system, and (b) the subsurface underlying such a surface location. Table 1 (Appendix A) referred to in the preceding quote is reproduced here as Table 1.

Associated with Table 1 (App. A) of Ref. 1 are instructions for converting a radionuclide release to the accessible environment over 10,000 yr (units: Ci) to a normalized release (units: dimensionless) for different types of radioactive waste. For transuranic waste, which is the waste category considered in this presentation, the normalized release nR is defined by

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

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

Radionuclide	Release Limit L_i per 1000 MTHM ^a or other unit of waste ^b
Americum	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 years	100
Any other radionuclide with a half-life greater than 20 years that does not emit alpha particles	1,000

- 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 years.

where

Q_i = cumulative release of radionuclide i to the accessible environment during the 10,000-yr period following closure of the repository (Ci),

L_i = release limit for radionuclide i given in Table 1 (Ci),

C = amount of transuranic waste emplaced in the repository (Ci).

The preceding normalization provides a way to reduce the effects of releases involving a variety of radionuclides to a single number.

Assessing compliance with 191.13 presents an interesting conceptual and computational problem due to the involvement of two different types of uncertainty. Requirement 191.13(a) specifies that the complementary cumulative distribution function (CCDF) for normalized radionuclide release to the accessible environment shall fall below a boundary line defined by the points (1, 0.1) and (10, 0.001) as indicated in Fig. 1. As such, 191.13(a) is an

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

example of the Farmer limit line approach to the definition of acceptable risk.³⁻⁵ The uncertainty characterized by the CCDF associated with 191.13(a) arises because a waste disposal site could experience a variety of different disruptions and is often referred to as stochastic uncertainty. Requirement 191.13(b) specifies that performance assessments should provide "a reasonable expectation" that compliance with 191.13(a) will be achieved. The "reasonable expectation" associated with 191.13(b) arises from an assessment of how much uncertainty there is with respect to where the CCDF in 191.13(a) is actually located. The uncertainty addressed in 191.13(b) arises from a lack of knowledge on the part of the analysts attempting to assess compliance with 191.13(a) and is often referred to as subjective uncertainty. The importance of separating the effects of stochastic and subjective uncertainty, as specified in 191.13, has been emphasized by a number of authors.⁶⁻¹⁶

The characterization of stochastic and subjective uncertainty involves the use of probability. Three entities are involved in a formal definition of probability: (1) a set S that contains everything that could occur for the particular "universe" under construction, (2) a suitably restricted set $\mathcal{S}$ of subsets of S , called a Borel or σ -algebra, and (3) a function p defined for elements of $\mathcal{S}$ that actually defines probability.¹⁷⁻¹⁹ Collectively, the triple $(S, \mathcal{S}, p)$ is called a probability space. In the terminology of probability theory, S is the sample space, the elements of S are elementary events, and the subsets of S contained in $\mathcal{S}$ are events. The probability space $(S_{st}, \mathcal{S}_{st}, p_{st})$ associated with stochastic uncertainty gives rise to the CCDF specified in 191.13(a), and the probability space $(S_{su}, \mathcal{S}_{su}, p_{su})$ associated with subjective uncertainty determines whether or not there is a "reasonable expectation" that 191.13(a) will be met as required by 191.13(b). In practice, a full measure-theoretic development of probability¹⁷⁻¹⁹ is never performed in a PA for a complex system. However, it is useful to introduce the idea of a probability space to emphasize that two internally-consistent developments of probability underly the treatment of stochastic and subjective uncertainty.

Preliminary performance assessments (PAs) conducted for the Waste Isolation Pilot Plant (WIPP) in 1991²⁰⁻²³ and 1992²⁴⁻²⁸ have used an experimental design based on importance sampling (Ref. 29, Sect. 5.4) to investigate the probability space for stochastic uncertainty and construct the CCDF specified in 191.13(a) and a random design based on Latin hypercube sampling^{30,31} to investigate the probability space for subjective uncertainty and assess the "reasonable expectation" called for in 191.13(b). This presentation will describe a Monte Carlo procedure that can be used to investigate stochastic uncertainty in PAs for the WIPP instead of the previously used importance sampling procedure. Desirable features of this Monte Carlo procedure include conceptual simplicity, computational efficiency, increased resolution on scenario probability, and better estimates of normalized releases to the accessible environment.

The presentation is organized as follows. The procedures used in the 1991 and 1992 WIPP PAs to treat stochastic and subjective uncertainty are described in Sect. 2. This description also introduces much of the notation and the mechanistic calculations that are needed to describe and illustrate the Monte Carlo procedure. The Monte Carlo construction of CCDFs is then presented in Sect. 3 and results of such constructions are compared with results obtained in the 1991 WIPP PA. The use of Monte Carlo procedures to estimate probabilities for certain complex scenarios involving pressurized brine pockets (i.e., E1E2-scenarios in a commonly-used WIPP terminology) is discussed in Sect. 4. Finally, a concluding discussion and prospectus on possible uses of Monte Carlo procedures for CCDF construction are given in Sect. 5.

2. CCDF Construction in 1991 and 1992 WIPP PAs

In the 1991 and 1992 WIPP PAs, the probability space $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ for stochastic uncertainty is defined by the following assumptions: (1) exploratory drilling for natural resources constitutes the only disruption at the WIPP with sufficient likelihood to be retained in the analysis (Ref. 21, Chapt. 3), (2) drilling intrusions follow a Poisson process³²⁻³⁵ with a rate term λ , (3) waste is partitioned into five activity levels (Ci/m²) with a probability of pL_i that a randomly placed borehole will intersect waste of activity level i (Ref. 22, Table 3.4-11), and (4) a fraction fPB_l of waste panel l (Fig. 2) is underlain by pressurized brine (Ref. 22, Sect. 5.1.1). In this development, the sample space $\mathcal{S}_{st}$ is

$$\mathcal{S}_{st} = \{x: x \text{ a single 10,000 yr history beginning at the decommissioning of the WIPP}\}. \quad (2)$$

Further, the set $\mathcal{J}_{st}$ and function p_{st} were never fully developed. Rather, as described below and in more detail elsewhere,³⁶ an importance sampling procedure was used to subdivide $\mathcal{S}_{st}$, with only those elements of $\mathcal{J}_{st}$ used in this importance sampling procedure being defined and assigned probabilities.

The importance sampling procedure used in the 1991 and 1992 WIPP PAs to subdivide $\mathcal{S}_{st}$ is based on the division of the 10,000-yr time period specified in 191.13(a) into a sequence

$$[t_{i-1}, t_i], \quad i = 1, 2, \dots, nT, \quad (3)$$

of disjoint time intervals. When the activity levels of the waste are not considered, these time intervals lead to subsets of $\mathcal{S}_{st}$ defined by

$$\mathcal{S}(\mathbf{n}) = \{x: x \text{ an element of } \mathcal{S}_{st} \text{ for which exactly } n(i) \text{ intrusions occur in time interval } [t_{i-1}, t_i] \text{ for } i = 1, 2, \dots, nT\} \quad (4)$$

and

$$\mathcal{S}^{+-}(t_{i-1}, t_i) = \{x: x \text{ an element of } \mathcal{S}_{st} \text{ for which two or more boreholes penetrate the same waste panel during the time interval } [t_{i-1}, t_i], \text{ with at least one of these boreholes penetrating a pressurized brine pocket (+) and at least one not penetrating a pressurized brine pocket (-)}\}, \quad (5)$$

where

$$\mathbf{n} = [n(1), n(2), \dots, n(nT)]. \quad (6)$$

In the 1991 WIPP PA, $nT = 5$ and each time interval $[t_{i-1}, t_i]$ had a length of 2000 yrs. In the 1992 WIPP PA, the intervals $[t_{i-1}, t_i]$ were defined in two different ways. To represent releases due to cuttings removal, $nT = 6$ and the individual intervals are [0, 150 yr], [150, 200 yr], [200, 500 yr], [500, 1500 yr], [1500, 4500 yr] and [4500,

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Fig. 2. Location of Waste Disposal Panels at the WIPP.

10,000 yr]; to represent releases due to groundwater transport, $nT = 2$ and the individual time intervals are $[0, 2000 \text{ yr}]$ and $[2000, 10,000 \text{ yr}]$.

When the activity levels of the waste are considered for the calculation of cuttings removal, the preceding time intervals lead to scenarios defined by

$$\mathcal{S}(\mathbf{l}, \mathbf{n}) = \{x: x \text{ an element of } \mathcal{S}(\mathbf{n}) \text{ for which the } j^{\text{th}} \text{ borehole encounters waste of activity level } l(j) \text{ for } j = 1, 2, \dots, nBH, \text{ where } nBH \text{ is the total number of boreholes associated with a time history in } \mathcal{S}(\mathbf{l}, \mathbf{n})\} \quad (7)$$

and

$$\mathcal{S}^{+-}(\mathbf{l}; t_{i-1}, t_i) = \{x: x \text{ an element of } \mathcal{S}^{+-}(t_{i-1}, t_i) \text{ for which the } j^{\text{th}} \text{ borehole encounters waste of activity level } l(j) \text{ for } j = 1, 2, \dots, nBH, \text{ where } nBH \text{ is the total number of boreholes associated with a time history in } \mathcal{S}^{+-}(\mathbf{l}; t_{i-1}, t_i)\}, \quad (8)$$

where

$$\mathbf{l} = [l(1), l(2), \dots, l(nBH)] \text{ and } nBH = \sum_{i=1}^{nT} n(i). \quad (9)$$

The sets $\mathcal{S}(\mathbf{l}, \mathbf{n})$ and $\mathcal{S}^{+-}(\mathbf{l}; t_{i-1}, t_i)$ were used as the strata (i.e., subsets of $\mathcal{S}_{st}$) in the importance sampling procedure used to incorporate stochastic uncertainty into the 1991 and 1992 WIPP PAs. The preceding sets are referred to as scenarios in most of the published literature relating to the 1991 and 1992 WIPP PAs (e.g., Refs. 27, 35-38); however, they will usually be referred to as strata in this presentation to emphasize that the procedures in use are a form of importance sampling.

The probabilities $pS(\mathbf{n})$ and $pS(\mathbf{l}, \mathbf{n})$ for $\mathcal{S}(\mathbf{n})$ and $\mathcal{S}(\mathbf{l}, \mathbf{n})$ are given by

$$pS(\mathbf{l}, \mathbf{n}) = \left\{ \prod_{j=1}^{nBH} \left[\frac{\lambda^{n(i)} (t_i - t_{i-1})^{n(i)}}{n(i)!} \right] \right\} \exp[-\lambda(t_{nT} - t_0)] \quad (10)$$

and

$$pS(\mathbf{l}, \mathbf{n}) = \left(\prod_{j=1}^{nBH} pL_{l(j)} \right) pS(\mathbf{n}) \quad (11)$$

under the assumption that the occurrence of boreholes through the repository follows a Poisson process with a rate constant λ (Ref. 21, Chapt. 2; Ref. 35), where $\mathbf{n}$ and $\mathbf{l}$ are defined in Eqs. (6) and (9), respectively, and pL_l is the probability that a randomly placed borehole through a waste panel will encounter waste of activity level l .

The probabilities $pS^{+-}(t_{i-1}, t_i)$ and $pS^{+-}(\mathbf{l}; t_{i-1}, t_i)$ for $\mathcal{S}^{+-}(t_{i-1}, t_i)$ and $\mathcal{S}^{+-}(\mathbf{l}; t_{i-1}, t_i)$ are given by

$$pS^{+-}(t_{i-1}, t_i) \doteq \sum_{l=1}^{nP} \left\{ 1 - \exp[-\alpha_l(t_i - t_{i-1})] \right\} \left\{ 1 - \exp[-\beta_l(t_i - t_{i-1})] \right\} \quad (12)$$

and

$$pS^{+-}(\mathbf{l}; t_{i-1}, t_i) \doteq \left(\prod_{j=1}^{nBH} pL_{l(j)} \right) pS^{+-}(t_{i-1}, t_i), \quad (13)$$

where

$$\alpha_l = aBP_l \lambda / aTOT$$

$$\beta_l = (aTOT_l - aBP_l) \lambda / aTOT$$

aBP_l = area (m²) of pressurized brine pocket under waste panel l ,

$aTOT_l$ = area (m²) of waste panel l ,

$aTOT$ = area (m²) of all waste panels,

nP = number of waste panels.

As illustrated in Fig. 2, the current design for the WIPP involves $nP = 10$ waste panels. For the 1991 and 1992 WIPP PAs, $aTOT_l$ and aBP_l were assumed to be the same for all waste panels. Thus,

$$aTOT_l = aTOT/nP \text{ and } aBP_l = fBP aTOT, \quad (14)$$

where

$$fBP = \sum_{l=1}^{nP} aBP_l / aTOT. \quad (15)$$

The expressions in Eqs. (11) and (12) are approximations, rather than exact formulas, for the probabilities $pS^{+-}(t_{i-1}, t_i)$ and $pS^{+-}(\mathbf{l}; t_{i-1}, t_i)$ (Ref. 21, Chapt. 2; Ref. 35). As will be discussed later, one of the reasons for using a Monte Carlo procedure for CCDF construction is to obtain better approximations to these probabilities.

The probabilities $pS(\mathbf{l}, \mathbf{n})$ and $pS^{+-}(\mathbf{l}; t_{i-1}, t_i)$ were used as the strata probabilities in the importance sampling procedure used in the 1991 and 1992 WIPP PAs.

The 1991 and 1992 WIPP PAs used the Kaplan/Garrick ordered triple representation for risk⁷ to express the connection between the importance sampling procedure in use and the CCDF required in 191.13(a). In this representation, risk is defined to be a set $\mathcal{R}$ of the form

$$\mathcal{R} = \{ (\mathcal{S}_i, p\mathcal{S}_i, \mathbf{cS}_i), i = 1, \dots, nS \}, \quad (16)$$

where

$\mathcal{S}_i$ = a set of similar occurrences,

$p\mathcal{S}_i$ = probability that an occurrence in the set $\mathcal{S}_i$ will take place,

$\mathbf{cS}_i$ = a vector of consequences associated with $\mathcal{S}_i$,

nS = number of sets selected for consideration.

Further, the sets $\mathcal{S}_i$ have no occurrences in common and $\mathcal{S}_{st} = \cup_i \mathcal{S}_i$. In the context of the importance sampling procedure used in the 1991 and 1992 WIPP PAs, the $\mathcal{S}_i$ are the strata associated with the design (i.e., $\mathcal{S}(\mathbf{l}, \mathbf{n})$ and $\mathcal{S}^{+-}(\mathbf{l}; t_{i-1}, t_i)$), and the $p\mathcal{S}_i$ are the strata probabilities (i.e., $p\mathcal{S}(\mathbf{l}, \mathbf{n})$ and $p\mathcal{S}^{+-}(\mathbf{l}; t_{i-1}, t_i)$). The vector $\mathbf{cS}_i$ contains environmental releases for individual isotopes, the normalized EPA release summed over all isotopes (Eq. (1)), and possibly other information associated with $\mathcal{S}_i$. As indicated in Fig. 3, each consequence cS contained in $\mathbf{cS}$ leads to a CCDF. When cS is the normalized EPA release summed over all isotopes, the CCDF required in 191.13(a) is obtained.

In the 1991 WIPP PA, the consequence vectors $\mathbf{cS}_i$ in Eq. (16) were determined in a sequence of calculations involving the computer programs CUTTINGS (Ref. 21, Chapt. 7; Ref. 39), BRAGFLO (Ref. 21, Chapt. 5), PANEL (Ref. 21, Chapt. 5), SECO2D (Ref. 21, Chapt. 6; Ref. 40) and STAFF2D (Ref. 21, Chapt. 6; Ref. 41) as indicated in Fig. 4. An overview of the mathematical models incorporated into these programs and used in the 1991 WIPP PA is presented in Sect. 3 of Helton et al.³⁸ The same sequence of models was also used in the 1992 WIPP PA with the exception that the SECO-TRANSPORT model (Ref. 25, Chapt. 7, App. C) was used instead of the STAFF2D to represent radionuclide transport in the Culebra Dolomite.

The importance sampling procedure used in the 1991 and 1992 WIPP PAs leads to too many strata to perform a detailed calculation for each strata with the models in Fig. 4. Rather, it is necessary to perform detailed release calculations for a relatively small number of strata and then to use these calculations to construct the releases associated with the remaining strata. In particular, the following results can be calculated for the time intervals $[t_{i-1}, t_i]$, $i = 1, \dots, nT$, in Eq. (3):

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Fig. 3. Construction of a CCDF from the Kaplan/Garrick Ordered Triple Representation for Risk. The S_i are assumed to be ordered so that $cS_i \leq cS_{i+1}$, $i = 1, 2, \dots, nS-1$, for the particular consequence cS under consideration.

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Fig. 4. Computer programs used in 1991 WIPP PA.

rC_i = EPA normalized release to the surface environment for cuttings removal due to a single borehole in time interval i with the assumption that the waste is homogeneous (i.e., wastes of different activity levels are not present), (17)

rC_{il} = EPA normalized release to the surface environment for cuttings removal due to a single borehole in time interval i that penetrates waste of activity level l , (18)

$rGWl_i$ = EPA normalized release to the accessible environment due to groundwater transport initiated by a single borehole in time interval i (i.e., an E2-type scenario), (19)

$rGW2_i$ = EPA normalized release to the accessible environment due to groundwater transport initiated by two boreholes in the same waste panel in time interval i , of which one penetrates a pressurized brine pocket and one does not (i.e., an E1E2-type scenario), (20)

with the assumption that the intrusions occur at the midpoints of the time intervals (e.g., at 1000, 3000, 5000, 7000 and 9000 yrs in the 1991 WIPP PA).

The normalized releases rC_i , rC_{il} and $rGWl_i$ can be used to construct the EPA normalized releases for $S(\mathbf{n})$ and $S(\mathbf{l}, \mathbf{n})$. For $S(\mathbf{n})$, the normalized release to the accessible environment $cS(\mathbf{n})$ is given by

$$cS(\mathbf{n}) = \sum_{j=1}^{nBH} (rC_{m(j)} + rGWl_{m(j)}), \quad (21)$$

where $m(j)$ designates the time interval in which the j^{th} borehole occurs. The vector

$$\mathbf{m} = [m(1), m(2), \dots, m(nBH)] \quad (22)$$

is uniquely determined once the vector $\mathbf{n}$ appearing in the definition of $S(\mathbf{n})$ is specified. Further, the normalized release to the accessible environment $cS(\mathbf{l}, \mathbf{n})$ for $S(\mathbf{l}, \mathbf{n})$ is given by

$$cS(\mathbf{l}, \mathbf{n}) = \sum_{j=1}^{nBH} (rC_{m(j), l(j)} + rGWl_{m(j)}). \quad (23)$$

Similarly, the normalized releases to the accessible environment $cS^{+-}(t_{i-1}, t_i)$ and $cS^{+-}(\mathbf{l}; t_{i-1}, t_i)$ for $S^{+-}(t_{i-1}, t_i)$ and $S^{+-}(\mathbf{l}; t_{i-1}, t_i)$ can be approximated by

$$cS^{+-}(t_{i-1}, t_i) = 2rC_i + rGW2_i. \quad (24)$$

and

$$cS^{+-}(\mathbf{l}; t_{i-1}, t_i) = \sum_{j=1}^2 rC_{i, l(j)} + rGW2_i, \quad (25)$$

respectively. Once the $cS(\mathbf{l}, \mathbf{n})$ and $cS^{+}(\mathbf{l}; t_{i-1}, t_i)$ are determined, the CCDF for comparison with the EPA release limits can be constructed as indicated in Fig. 3.

So far, this section has outlined the importance sampling procedure used to incorporate stochastic uncertainty into the 1991 and 1992 WIPP PAs. Subjective uncertainty enters the analysis when parameter values must be selected and various other decisions made in the quantification of the risk representation $\mathcal{R}$ in Eq. (16). Specifically, $\mathcal{R}$ can be viewed as a function of the form

$$\mathcal{R}(\mathbf{x}) = \{[\mathcal{S}_i(\mathbf{x}), p\mathcal{S}_i(\mathbf{x}), c\mathcal{S}_i(\mathbf{x})], i = 1, \dots, n\mathcal{S}(\mathbf{x})\}, \quad (26)$$

where

$$\mathbf{x} = [x_1, x_2, \dots, x_{nI}] \quad (27)$$

is a vector of inputs required in the determination of $\mathcal{R}$ and thus in the determination of the CCDF specified in 191.13(a). Lack of knowledge about the appropriate value to use for $\mathbf{x}$ is subjective uncertainty and is characterized by the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ for subjective uncertainty.

In the 1991 and 1992 WIPP PAs, the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ for subjective uncertainty was defined by specifying distributions

$$D_1, D_2, \dots, D_{nI} \quad (28)$$

for the elements of $\mathbf{x}$, where D_j is the distribution for x_j . These distributions characterize subjective uncertainty and indicate a degree of belief as to where the appropriate value to use for each variable is located. Specifically, the sample space $\mathcal{S}_{su}$ for subjective uncertainty consists of all possible values for $\mathbf{x}$, and the definitions of $\mathcal{J}_{su}$ and p_{su} follow from the D_j . The 1991 WIPP PA considered $nI = 45$ imprecisely-known variables (Ref. 22, Tables 6.0-1, 6.0-2, 6.0-3; also, Ref. 37, Table VIII and Ref. 38, Table 8). The variables contained in $\mathbf{x}$ for the 1992 WIPP PA were modified slightly, with a total of $nI = 49$ variables contained in $\mathbf{x}$ (Ref. 26, Tables 6.0-1, 6.0-2, 6.0-3; Ref. 27, Table 3-1). As some of the variables contained in $\mathbf{x}$ affect the definition of the probability space for stochastic uncertainty (e.g., the rate constant λ in the Poisson model for drilling intrusions), this space is actually a function $[\mathcal{S}_{st}(\mathbf{x}), \mathcal{J}_{st}(\mathbf{x}), p_{st}(\mathbf{x})]$ of $\mathbf{x}$.

The 1991 and 1992 WIPP PAs used a random design to incorporate the probability space for subjective uncertainty into the analysis to show compliance with 191.13 and, in particular, to satisfy the "reasonable expectation" requirement in 191.13(b). Specifically, Latin hypercube sampling^{30,31} was used to generate a sample

$$\mathbf{x}_k, \quad k = 1, 2, \dots, nK, \quad (29)$$

from the $\mathbf{x}$ (i.e., from $\mathcal{S}_{su}$) according to the distributions indicated in Eq. (28). Further, the Iman/Conover restricted pairing technique⁴² was used to induce specified correlations between correlated variables and to assure that uncorrelated variables had correlations close to zero. Sample sizes of $nK = 60$ and $nK = 70$ were used in the 1991 and 1992 WIPP PAs, respectively.

A random design, and Latin hypercube sampling in particular, was selected as the experimental design for subjective uncertainty for several reasons (Ref. 43, Sect. 2.6): (1) efficient stratification across the full range of each variable, (2) ease of incorporation of correlations, (3) computational efficiency, (4) ease of implementation, (5) conceptual simplicity, (6) facilitation of sensitivity analysis, and (7) observed robustness in past studies (Refs. 44-46). In contrast, the high dimensionality of $\mathcal{S}_{su}$ (i.e., $\mathcal{S}_{su}$ is a subset of R^{45} and R^{49} in the 1991 and 1992 WIPP PAs, respectively) and associated correlation structure make importance sampling and classical experimental designs (e.g., fractional factorial, central composite, ...) unlikely candidates for the incorporation of subjective uncertainty.

Evaluation of $\mathcal{R}$ for the sample elements $\mathbf{x}_k$ in Eq. (20) leads to the sequence of results

$$\mathcal{R}(\mathbf{x}_k) = \left\{ \left[\mathcal{S}_i(\mathbf{x}_k), p_{\mathcal{S}_i}(\mathbf{x}_k), \mathbf{cS}_i(\mathbf{x}_k) \right], i = 1, \dots, nS(\mathbf{x}_k) \right\} \quad (30)$$

for $k = 1, \dots, nK$. For a given set $\mathcal{R}(\mathbf{x}_k)$, each consequence result $\mathbf{cS}$ contained in the vectors $\mathbf{cS}_i(\mathbf{x}_k)$ leads to a CCDF as shown in Fig. 3 that displays the effect of stochastic uncertainty (i.e., this CCDF derives from the probability space $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$ or, more explicitly, the probability space $[\mathcal{S}_{st}(\mathbf{x}_k), \mathcal{J}_{st}(\mathbf{x}_k), p_{st}(\mathbf{x}_k)]$). In turn, consideration of all the $\mathcal{R}(\mathbf{x}_k)$ leads to a distribution of CCDFs for each consequence result that displays the effect of subjective uncertainty (i.e., this distribution of CCDFs derives from the probability space $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ for subjective uncertainty). As an example, the distributions of CCDFs for normalized release to the accessible environment due to cuttings removal and groundwater transport obtained in the 1991 WIPP PA are shown in Fig. 5. The individual CCDFs in this figure result from stochastic uncertainty, while the distributions of CCDFs result from subjective uncertainty. It is the location of the distribution of CCDFs in Fig. 5 relative to the limit line specified in 191.13(a) that is providing information on the "reasonable expectation" required in 191.13(b) that 191.13(a) will be met. In particular, the appearance of all or most of the CCDFs in distributions of the form shown in Fig. 5 is indicative of a "reasonable expectation" that 191.13(a) will be met.

Results obtained in the analysis that lead to the CCDFs in Fig. 5 will be used to illustrate the Monte Carlo procedure for CCDF construction presented in the next section. In particular, results obtained for sample element 46 in the 1991 WIPP PA will be used as this sample element was previously used to illustrate the importance sampling procedure summarized in this section.^{35,36} For future reference, CCDFs constructed for this sample element are shown in Fig. 6. This construction used the activity level probabilities in Table 2 and the normalized releases in Table 3. Further, the rate constant λ in the Poisson model for drilling intrusions in Eqs. (10) and (12) and the brine

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Fig. 5. Distribution of CCDFs for normalized release to the accessible environment due to cuttings removal (left frame) and groundwater transport (right frame) obtained in the 1991 WIPP PA (Ref. 36, Figs. 1 and 2).

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Fig. 6. Estimated CCDFs for sample element 46 (Ref. 36, Fig. 4).

Table 2. Projected Activity Levels (Ci/m²) in Waste That Is Currently Stored and May Be Shipped to the WIPP (Ref. 35, Table 5; based on the Table 3.4-11 of Ref. 22)

Activity level	Type ^a	Probability ^b	Time (years)					
			0	1000	3000	5000	7000	9000
1	CH	0.402 3	3.483 3	0.271 8	0.184 0	0.168 8	0.157 5	0.147 3
2	CH	0.299 8	34.832 6	2.717 7	1.840 1	1.687 5	1.574 8	1.472 9
3	CH	0.224 2	348.326	27.177	18.401	16.875	15.748	14.729
4	CH	0.014 9	3483.26	271.77	184.01	168.75	157.48	147.29
5	RH	0.058 8	117.671 7	0.154 6	0.121 2	0.113 9	0.108 2	0.103 0
Average for CH waste:			150.790 5	11.764 8	7.965 8	7.305 3	6.817 4	6.376 4

^a CH designates contact-handled waste; RH designates remote-handled waste.

^b Probability pL_l that a randomly placed borehole through the waste panels will intersect waste of activity level l , $l = 1, 2, 3, 4, 5$.

Table 3. Normalized Radionuclide Releases Used to Illustrate Scenario Construction Procedures (Ref. 36, Table 4)

Time ^a	$rGW1_i^b$	$rGW2_i^c$	rC_i^d	rC_{il}^e	rC_{i2}^e	rC_{i3}^e	rC_{i4}^e	rC_{i5}^e
1000 yr	9.92E-06	1.48E-05	6.96E-03	1.71E-04	1.71E-03	1.71E-02	1.71E-01	9.71E-05
3000 yr	2.51E-06	5.08E-06	4.72E-03	1.16E-04	1.16E-03	1.16E-02	1.16E-01	7.61E-05
5000 yr	3.61E-07	1.34E-06	4.33E-03	1.06E-04	1.06E-03	1.06E-02	1.06E-01	7.16E-05
7000 yr	7.72E-08	3.16E-07	4.04E-03	9.92E-05	9.92E-04	9.92E-03	9.92E-02	6.80E-05
9000 yr	0.00E+00	5.08E-08	3.78E-03	9.28E-05	9.28E-04	9.28E-03	9.28E-02	6.47E-05

The releases presented in this table were calculated for sample element 46 in the 1991 WIPP PA (see Ref. 21, Appendix B).

^a Time at which intrusion occurs.

^b EPA normalized release (dimensionless) to the accessible environment for groundwater transport (with a dual porosity model in the Culebra Dolomite) initiated by a single borehole in time interval i (i.e., an E2-type intrusion).

^c EPA normalized release (dimensionless) to the accessible environment for groundwater transport (with a dual porosity model in the Culebra Dolomite) initiated by two boreholes in the same waste panel in time interval i , of which one penetrates a pressurized brine pocket and one does not (i.e., an E1E2-type intrusion).

^d EPA normalized release (dimensionless) to the surface environment for cuttings removal as a result of a single borehole in time interval i with the assumption that the waste is homogeneous (i.e., waste of various activity levels is not present). Calculation of the rC_i used the average activity level shown in Table 2.

^e EPA normalized release (dimensionless) to the surface environment for cuttings removal as a result of a single borehole in time interval i that penetrates waste of activity level l . Calculation of the rC_{il} used the activity levels corresponding to $l = 1, 2, 3, 4, 5$ shown in Table 2.

pocket area fraction fBP in Eq. (15) were uncertain inputs in the 1991 WIPP PA, with assigned values of $\lambda = 8.4424 \times 10^{-5} \text{ yr}^{-1}$ and $fBP = 0.44981$ for sample element 46.

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3. Monte Carlo Procedure for CCDF Construction

Monte Carlo procedures provide an alternative to the importance sampling procedure described in the preceding section for the construction of the CCDF specified in 191.13(a). With such procedures, elements of the sample space $\mathcal{S}_{st}$ are randomly sampled and the associated releases to the accessible environment are estimated. This produces a sequence of results of the form

$$(x_i, \mathbf{cS}_i), i = 1, 2, \dots, nRS, \quad (31)$$

where

x_i = randomly selected element of $\mathcal{S}_{st}$,

$\mathbf{cS}_i$ = vector of consequences associated with x_i ,

nRS = number of random samples taken from $\mathcal{S}_{st}$.

As in the importance sampling procedure indicated in Eq. (16), the vector $\mathbf{cS}_i$ would typically contain a variety of quantities, including the normalized releases to the accessible environment required in conjunction with 191.13(a). The number of samples nRS could possibly be quite large (e.g., on the order of 10^5 or larger). Once the results in Eq. (31) are generated, CCDFs for the elements of $\mathbf{cS}$ can be constructed as shown in Fig. 3. The probabilities pS_i in this construction are given by

$$pS_i = 1/nRS \quad (32)$$

when random sampling is used to select the x_i from $\mathcal{S}_{st}$. As done in the preceding sentence, it is sometimes semantically convenient to refer to $1/nRS$ as the probability for x_i ; however, this is not technically correct when the x_i are generated by random sampling. Each x_i has a probability of zero; $1/nRS$ is not the probability of x_i , but rather a weight that can be used to estimate distributions and other quantities (e.g., a mean) associated with the x_i .

Two obvious questions arise in the implementation of the Monte Carlo procedure indicated in Eq. (31): "How to sample the x_i from $\mathcal{S}_{st}$?", and "How to obtain the consequence vectors $\mathbf{cS}_i$?". Each of these questions is now addressed.

How to sample the x_i is addressed first. As indicated in Eq. (2), each element x of $\mathcal{S}_{st}$ contains a description of a possible 10,000 yr sequence of occurrences at the WIPP. In this analysis, drilling intrusions are the only occurrences under consideration. Thus, each element of $\mathcal{S}_{st}$ is defined by the number of drilling intrusions that occur, the time of each drilling intrusion, the location of each drilling intrusion, and the activity level of the waste encountered by each drilling intrusion. Thus, each element x of $\mathcal{S}_{st}$ is characterized by a vector $\mathbf{c}(x)$ of the form

$$\mathbf{c}(x) = [tBH_1, xBH_1, aBH_1, tBH_2, xBH_2, aBH_2, \dots, tBH_{nBH}, xBH_{nBH}, aBH_{nBH}] \quad (33)$$

where

tBH_j = time (yr) at which the j^{th} drilling intrusion occurs,

xBH_j = location of the j^{th} drilling intrusion,

aBH_j = activity level of waste (Ci/m²) penetrated by the j^{th} drilling intrusion,

nBH = number of drilling intrusions,

and the times tBH_j are assumed to be ordered so that $tBH_j \leq tBH_{j+1}$ for $j = 1, 2, \dots, nBH-1$. In the preceding description, only one coordinate (i.e., xBH_j) is used to represent the location of a drilling intrusion due to the rectilinear nature of the waste panels at the WIPP (Fig. 2) and the current level of resolution used in BRAGFLO to model gas and brine behavior in a waste panel. The use of two coordinates (i.e., xBH_j and yBH_j) to represent the location of a drilling intrusion is also possible if such resolution is appropriate for the models used to represent the physical processes associated with x .

Once an element of $\mathcal{S}_{st}$ is represented as a vector of the form in Eq. (33), sampling from $\mathcal{S}_{st}$ becomes an exercise in randomly sampling numbers from the interval [0, 1]. The manner in which such sampling can be done to produce the vector $\mathbf{c}(x)$, and hence an element of x of $\mathcal{S}_{st}$, is not unique. The following outlines one possible procedure.

With the assumption that drilling intrusions follow a Poisson process with a rate constant λ , the probability $prob(n)$ that exactly n drilling intrusions occur in the time interval $[t_0, t_{nT}]$ is given by

$$prob(n) = \left[(t_{nT} - t_0)^n \lambda^n / n! \right] \exp \left[-(t_{nT} - t_0) \lambda \right]. \quad (34)$$

In PAs for the WIPP, $t_0 = 100$ yr due to the assumption of 100 yr of administrative control and $t_{nT} = 10,000$ yr as specified in 191.13(a). The value for nBH in Eq. (33) can be obtained by randomly sampling a number r from the interval [0, 1] and then assigning nBH the smallest integer value for which the inequality

$$r \leq \sum_{n=0}^{nBH} prob(n) \quad (35)$$

is satisfied.

Once a value for nBH is selected, an additional $3 nBH$ random numbers can be used to assign the values for tBH_j , xBH_j and aBH_j , $j = 1, 2, \dots, nBH$. Specifically, let $rtBH_j$, $rxBH_j$ and $raBH_j$, $j = 1, 2, \dots, nBH$, represent numbers randomly selected from the interval [0, 1]. Then, the tBH_j are defined by

$$tBH_j = t_0 + rtBH_j(t_{nT} - t_0), \quad (36)$$

where $t_0 = 100$ yr and $t_{nT} = 10,000$ yr in recent WIPP PAs. Similarly, the xBH_j are defined by

$$xBH_j = rxBH_j aTOT, \quad (37)$$

where $aTOT$ is the total area (m^2) of the waste panels as defined in conjunction with Eqs. (12) and (13). Finally, aBH_j corresponds to penetration of waste of activity level m , where m is the smallest integer such that

$$raBH_j \leq \sum_{l=1}^m pL_l \quad (38)$$

and pL_l is the probability that a randomly placed drilling intrusion will penetrate waste of activity level l .

The definition of xBH_j in Eq. (37) permits the determination of both the waste panel penetrated by a drilling intrusion and whether or not a pressurized brine pocket is penetrated. Specifically, the j^{th} drilling intrusion penetrates waste panel m , where m is the smallest integer such that

$$xBH_j \leq \sum_{l=1}^m aTOT_l \quad (39)$$

and $aTOT_l$ is the area of waste panel l as defined in conjunction with Eqs. (12) and (13). Further, a pressurized brine pocket is penetrated when the inequality

$$\sum_{l=1}^{m-1} aTOT_l < xBH_j \leq aBP_m + \sum_{l=1}^{m-1} aTOT_l \quad (40)$$

is satisfied, where aBP_m is the area (m^2) of pressurized brine under waste panel m .

How to obtain consequence values, in particular normalized releases to the accessible environment, contained in the consequence vectors $\mathbf{cS}_i$ is now addressed. The large number of samples that will be required from $\mathcal{S}_{st}$ precludes the use of the models indicated in Fig. 4 to perform a release calculation for every x_i sampled from $\mathcal{S}_{st}$. Rather, it is necessary to perform a limited number of detailed calculations with the models indicated in Fig. 4 and then use the results of these calculations to construct the releases associated with the individual x_i . There is nothing novel in this. The same type of process was also needed in the importance sampling procedure described in the preceding section. Indeed, the example in this section will use the same release results (i.e., rC_i , rC_{il} , $rGWI_i$, $rGW2_i$ in Eqs. (17) - (20)) that underlie the example used to illustrate importance sampling.

The normalized release to the accessible environment $nR(x)$ for an element x of S_{st} is given by

$$nR(x) = nRC(x) + nRG(x), \quad (41)$$

where

$nRC(x)$ = normalized release to the accessible environment due to cuttings removal,

$nRG(x)$ = normalized release to the accessible environment due to groundwater transport.

The releases $nRC(x)$ and $nRG(x)$ can be determined separately and then summed to obtain $nR(x)$.

Definition of the cuttings release $nRC(x)$ is considered first. The assumption is made that no synergisms exist between the cuttings releases associated with individual drilling intrusions; specifically, the releases associated with individual drilling intrusions are assumed to be unaffected by any other drilling intrusions that may occur. When the effects of activity loading are included, $nRC(x)$ is defined by

$$nRC(x) = \sum_{j=1}^{nBH} rC_{m(j),l(j)} \quad (42)$$

with the vectors $\mathbf{l}$ and $\mathbf{m}$ defined for x as indicated in Eqs. (9) and (22), respectively. The preceding is the same as the cuttings component of the releases defined in Eqs. (23) and (25) for use with the importance sampling procedure. If the effects of activity loading are not included, $nRC(x)$ is defined by

$$nRC(x) = \sum_{j=1}^{nBH} rC_{m(j)}, \quad (43)$$

which is the same as the cuttings component of the releases defined in Eqs. (21) and (24) for use with the importance sampling procedure.

Definition of the groundwater release $nRG(x)$ is now considered. A number of assumptions as summarized in Table 4 are made to provide a basis for the use of the releases $rGW1_i$ and $rGW2_i$ in Eqs. (19) and (20) in the construction of a release $nRG(x)$ for an arbitrary element x from S_{st} . Assumption 1 implies that the releases from the individual waste panels can be considered separately. As a result, it is convenient to express $nRG(x)$ in the form

$$nRG(x) = \sum_{l=1}^{nP} nRG_l(x), \quad (44)$$

Table 4. Assumptions Used in Construction of Groundwater Release to the Accessible Environment $nRG(x)$ for an Arbitrary Element x of S_{st}

Assumption	Description
1	Waste panels are isolated in the sense that the releases that occur from one waste panel are unaffected by the drilling intrusions that may occur into other waste panels.
2	Single drilling intrusions that penetrate a pressurized brine pocket (i.e., an E1 intrusion in WIPP terminology) and single drilling intrusions that do not penetrate a pressurized brine pocket (i.e., an E2 intrusion in WIPP terminology) have the same releases. This may not be an appropriate assumption because the waste panel will fill with brine more rapidly for an E1 than an E2 intrusion (Ref. 37, Sect. IV.D). However, this assumption was made in the 1991 and 1992 WIPP PAs.
3	Multiple E1 intrusions into a waste panel have the same release as the single earliest intrusion. Similarly, multiple E2 intrusions into a waste panel have the same release as the single earliest intrusion. This assumption derives from the fact that brine from the Salado Formation transports radionuclides to an intruding borehole and multiple boreholes will not increase the amount of this brine available for radionuclide transport within a panel.
4	A release involving at least one drilling intrusion that penetrates a pressurized brine pocket and at least one drilling intrusion that does not penetrate a pressurized brine pocket (i.e., an E1E2 intrusion in WIPP terminology) begins at the earliest time at which both an E1 and an E2 intrusion have occurred.
5	An E1E2 intrusion into a waste panel involving more than 2 drilling intrusions has the same release as an E1E2 intrusion involving exactly 2 drilling intrusions. As in Assumption 3, this assumption derives from the amount of brine available for radionuclide transport within a waste panel.

where

$nRG_l(x)$ = normalized release to accessible environment associated with x due to groundwater transport for radionuclides originating from waste panel l .

The releases $nRG_l(x)$ can then be determined separately and summed to obtain $nRG(x)$. To facilitate this determination, let

$$\mathbf{v}_l(x) = [t_l(1), m_l(1), b_l(1), t_l(2), m_l(2), b_l(2), \dots, t_l(nBH_l), m_l(nBH_l), b_l(nBH_l)], \quad (45)$$

where

$t_l(j)$ = time (yr) at which the j^{th} drilling intrusion into waste panel l occurs,

$m_l(j) = i$ implies that the j^{th} drilling intrusion into waste panel l occurs in time interval $[t_{i-1}, t_i]$,

$$b_l(j) = \begin{cases} 1 & \text{if the } j^{\text{th}} \text{ drilling intrusion into waste panel } l \text{ penetrates a pressurized brine pocket} \\ 0 & \text{otherwise,} \end{cases}$$

nBH_l = number of drilling intrusions into waste panel l ,

and the intrusion times $t_f(j)$ are assumed to be ordered to that $t_f(j) \leq t_f(j+1)$ for $j = 1, 2, \dots, nBH_l - 1$. The vector $\mathbf{v}(x)$ can be constructed from information in the definition of $\mathbf{c}(x)$ in Eq. (33).

Four possibilities exist. First, $nBH_l = 0$. In this case, no groundwater release occurs and

$$nRG_l(x) = 0. \quad (46)$$

Second, $nBH_l \neq 0$ and all drilling intrusions penetrate a pressurized brine pocket (i.e., $b_l(j) = 1$ for $j = 1, 2, \dots, nBH_l$). Third, $nBH_l \neq 0$ and none of the drilling intrusions penetrate a pressurized brine pocket (i.e., $b_l(j) = 0$ for $j = 1, 2, \dots, nBH_l$). From Assumption 2 in Table 4, the two preceding cases will have the same release. Further, from Assumption 3, the release from the waste panel is the release for the earliest intrusion. Thus, the release for the two preceding cases is

$$nRG_l(x) = rGW I_{m_l(1)}. \quad (47)$$

Fourth, $nBH_l \geq 2$, at least one drilling intrusion penetrates a pressurized brine pocket (i.e., $b_l(j) = 1$ for at least one j) and at least one drilling intrusion does not penetrate a pressurized brine pocket (i.e., $b_l(j) = 0$ for at least one j). Let $jE1E2$ be the smallest integer such that the sequence $b_l(1), b_l(2), \dots, b_l(jE1E2)$ contains both 0's and 1's (i.e., $[t_0, t_f(jE1E2)]$ is the shortest time interval associated with x that includes at least one drilling intrusion that penetrates a pressurized brine pocket and at least one drilling intrusion that does not penetrate a pressurized brine pocket). The release for this case is approximated by

$$nRG_l(x) = \left(rGW I_{m_l(1)} - rGW I_{m_l(jE1E2)} \right) + rGW 2_{m_l(jE1E2)}. \quad (48)$$

The first term on the right in Eq. (48) is the release that takes place before the occurrence of an E1E2-type intrusion and derives from Assumptions 2 and 3. The second term on the right in Eq. (48) is the release that takes place after the occurrence of an E1E2-type intrusion and derives from Assumptions 4 and 5.

A Monte Carlo procedure for the construction of the CCDF specified in 191.13(a) has been described. The results for sample element 46 in the 1991 WIPP PA are now used to illustrate this procedure. Specifically, vectors of the form $\mathbf{c}(x)$ indicated in Eq. (33) are randomly selected with $\lambda = 8.4424 \times 10^{-5} \text{ yr}^{-1}$ (i.e., the value for λ in sample element 46), the waste panel areas in Table 5, and the activity level probabilities in Table 2. Once $\mathbf{c}(x)$ is obtained, the vectors $\mathbf{v}_f(x)$ in Eq. (45) are constructed. In this construction, a brine pocket area fraction of $fBP = 0.44981$ is used in consistency with the 1991 WIPP PA (see Eq. (15)), which is the sampled value for sample element 46. Given $\mathbf{c}(x)$ and $\mathbf{v}_f(x)$, the associated normalized releases $nR(x)$, $nRC(x)$, $nRG(x)$ and $nRG_f(x)$ are then

Table 5. Parameter Values Used in Example Calculation of Probabilities for E1E2-Type Scenarios (Ref. 35, Table 4; adapted from Table 5.1-1 of Ref. 22 with depth to pressurized brine assumed to be less than 1250 m)

	$aTOT_l^a$	aBP_l^b	$aBP_l / aTOT_l$
Panel 1	11 530	11 530	1.000 0
Panel 2	11 530	8 249	0.715 4
Panel 3	11 530	3 548	0.307 7
Panel 4	11 530	8 869	0.769 2
Panel 5	11 530	4 833	0.419 2
Panel 6	11 530	0	0.000 0
Panel 7	11 530	0	0.000 0
Panel 8	11 530	7 432	0.644 6
Southern panel	8 413	3 786	0.450 0
Northern panel	8 701	1 044	0.120 0

Additional values:

$$aTOT = \sum_{l=1}^{10} aTOT_l = 109\,354$$

$$aBP = \sum_{l=1}^{10} aBP_l = 49\,291$$

$$fBP = aBP / aTOT = 0.45075$$

^a $aTOT_l$ = area (m²) of waste panel l .

^b aBP_l = area (m²) of pressurized brine under waste panel l .

constructed from the results in Table 3 as indicated in Eqs. (41) - (48). The outcome of this procedure is a sequence of results of the form shown in Eq. (31). Due to the large number of samples in use (i.e., nRS), the results cS_i for the individual x_i sampled from S_{st} are not saved; instead, a binning procedure is used whereby the range of each release is subdivided into intervals and the number of releases falling into each interval is accumulated. This binning procedure was also used in the importance sampling procedure described in the preceding section due to the large number of strata involved.

As shown in Fig. 7, the importance sampling procedure implemented with the program CCDFPERM³⁶ described in Sect. 2 and the Monte Carlo procedure described in this section produce similar results. The CCDFs for cuttings removal for waste of average activity level are essentially identical. The CCDFs for cuttings removal for waste of different activity levels are also similar. There is some separation between the two CCDFs for groundwater transport because the Monte Carlo simulation is using a less restrictive definition of an E1E2-type intrusion. Specifically, the drilling intrusions that produce an E1E2-type intrusion are not required to fall in the time intervals [100, 2000 yr], [2000, 4000 yr], [4000, 6000 yr], [6000, 8000 yr] and [8000, 10,000 yr] used to define E1E2-type intrusions in the importance sampling procedure. In addition, the Monte Carlo procedure includes the

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Fig. 7. Estimated CCDFs for sample element 46 obtained with importance sampling and a Monte Carlo sample of size 5×10^5 .

release that takes place before the second borehole associated with an E1E2-type intrusion occurs, allows for the possibility that an E1E2-type intrusion may occur in conjunction with one or more E2-type intrusions for a given element of S_{st} , and also allows for the possibility that more than one E1E2-type intrusion may occur for a given element of S_{st} .

As shown in Fig. 8, the Monte Carlo procedure for CCDF construction has clearly converged with a sample of size 5×10^5 . Indeed, adequate resolution for comparison with the EPA release limits is obtained with a much smaller sample size (i.e., between 5×10^3 and 5×10^4). The evaluation of the three CCDFs in Fig. 8 with a sample of size 5×10^5 required approximately 27 s on a Digital Vax Alpha using VMS. Thus, the computational requirements associated with the Monte Carlo procedure for CCDF construction described in this presentation are quite reasonable. In particular, the computational cost associated with the Monte Carlo procedure is acceptable for the construction of distributions of CCDFs of the form shown in Fig. 5.

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Fig. 8. Estimated CCDFs for sample element 46 obtained with Monte Carlo samples of size 5×10^2 , 5×10^3 , 5×10^4 and 5×10^5 .

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4. Monte Carlo Estimation of Scenario Probabilities

Scenarios that involve E1E2-type intrusions are important in PAs for the WIPP because of the potentially large releases associated with these intrusions. Large releases may result because of brine flow up an intruding borehole from a pressurized brine pocket, through a waste panel, and then up a second borehole to the Culebra Dolomite. Such flow has the potential to access more of the radionuclide inventory in a waste panel than a single borehole or multiple boreholes that do not involve cross flow between the individual boreholes.

Due to the complexity of the problem (i.e., multiple waste panels, different areas of pressurized brine under individual waste panels, drilling intrusions at different times and locations), the derivation of exact formulas for the probability of scenarios that involve E1E2-type intrusions is difficult. Formulas such as the one given in Eq. (12) and used in 1991 and 1992 WIPP PAs are approximations whose accuracy is difficult to verify with analytic procedures. In contrast, Monte Carlo procedures of the type discussed in the preceding section provide a relatively simple means of obtaining accurate approximations of the probability of such scenarios.

Examples of probabilities for scenarios involving E1E2-type intrusions are shown in Table 6. Scenarios of the form $S^{+-}(t, t+\Delta t)$ are defined in Eq. (5) and involve intrusion of a waste panel during the time interval $[t, t+\Delta t]$ by two or more boreholes, with at least one of these boreholes penetrating a pressurized brine pocket and at least one of these boreholes not penetrating a pressurized brine pocket. For perspective, a scenario denoted by $S^+(t, t+\Delta t)$ is also considered, where

$$S^+(t, t+\Delta t) = \{x: x \text{ an element of } S_{st} \text{ for which two or more boreholes penetrate the same waste panel during the time interval } [t, t+\Delta t], \text{ with at least one of these boreholes penetrating a pressurized brine pocket}\}. \quad (49)$$

The scenarios $S^{+-}(t, t+\Delta t)$ and $S^+(t, t+\Delta t)$ differ in that only penetration of a pressurized brine pocket is required in the definition of $S^+(t, t+\Delta t)$. As examination of Table 6 shows, (1) the approximate formula in Eq. (12) for the probability of $S^{+-}(t, t+\Delta t)$ provides results close to those obtained in the Monte Carlo simulation, (2) probabilities for $S^+(t, t+\Delta t)$ are somewhat higher than those for $S^{+-}(t, t+\Delta t)$, (3) probabilities for $S^{+-}(t, t+\Delta t)$ can be large when the entire 9900 yr period is considered, (4) probabilities for $S^{+-}(t, t+\Delta t)$ are small when $\Delta t \leq 500$ yr, (5) the probability of $S^{+-}(t, t+\Delta t)$ decreases as λ increases, and (6) the use of panel-dependent brine pocket area fractions produces somewhat smaller probabilities for $S^{+-}(t, t+\Delta t)$ than the use of a single average brine pocket area fraction.

The probabilities in Table 6 are for the scenarios $S^{+-}(t, t+\Delta t)$ and $S^+(t, t+\Delta t)$ and thus involve drilling intrusions that occur within the time interval $[t, t+\Delta t]$. Another way to define scenarios that involve E1E2-type intrusions is on the basis of the time of separation between the drilling intrusions. Specifically, scenarios $S^{+-}(\Delta t)$ and $S^+(\Delta t)$ can be defined by

Table 6. Comparison of Probabilities for Scenarios Involving E1E2-Type Intrusions That Occur with Fixed Time Intervals for the Defining Boreholes

Time Interval [t, t+Δt]	$pS_A^{+-}(t, t+\Delta t)^a$ $\lambda=3.28 \times 10^{-4} \text{ yr}^{-1}$	$pS_M^{+-}(t, t+\Delta t)^b$ $\lambda=3.28 \times 10^{-4} \text{ yr}^{-1}$	$pS_M^{+}(t, t+\Delta t)^c$ $\lambda=3.28 \times 10^{-4} \text{ yr}^{-1}$	$pS_A^{+-}(t, t+\Delta t)$ $\lambda=8.44 \times 10^{-4} \text{ yr}^{-1}$	$pS_M^{+-}(t, t+\Delta t)$ $\lambda=8.44 \times 10^{-5} \text{ yr}^{-1}$	$pS_M^{+}(t, t+\Delta t)$ $\lambda=8.44 \times 10^{-5} \text{ yr}^{-1}$
Constant Brine Pocket Area Fraction: $fBP = 0.45075$ (Table 5)						
[t, t+100 yr]	2.69×10^{-5}	2.40×10^{-5d}	3.40×10^{-5}	1.78×10^{-6}	0.00	1.00×10^{-6}
[t, t+500 yr]	6.68×10^{-4}	6.20×10^{-4}	8.79×10^{-4}	4.45×10^{-5}	5.00×10^{-5}	6.60×10^{-5}
[t, t+1000 yr]	2.65×10^{-3}	2.61×10^{-3}	3.65×10^{-3}	1.78×10^{-4}	1.89×10^{-4}	2.49×10^{-4}
[t, t+2000 yr]	1.04×10^{-2}	1.02×10^{-2}	1.43×10^{-2}	7.08×10^{-4}	7.33×10^{-4}	9.85×10^{-4}
[t, t+5000 yr]	6.20×10^{-2}	6.00×10^{-2}	8.25×10^{-2}	4.37×10^{-3}	4.37×10^{-3}	6.11×10^{-3}
[t, t+9900 yr]	2.24×10^{-1}	2.02×10^{-1}	2.67×10^{-1}	1.68×10^{-2}	1.68×10^{-2}	2.34×10^{-2}
Panel-Dependent Brine Pocket Area Fractions: $fBP_i = aBP_i/aTOT_i$ (Table 5)						
[t, t+100 yr]	1.50×10^{-5}	1.00×10^{-5}	2.40×10^{-5}	9.96×10^{-7}	0.00	1.00×10^{-6}
[t, t+500 yr]	3.73×10^{-4}	3.74×10^{-4}	7.57×10^{-4}	2.49×10^{-5}	2.90×10^{-5}	5.60×10^{-5}
[t, t+1000 yr]	1.48×10^{-3}	1.46×10^{-3}	3.16×10^{-3}	9.92×10^{-5}	1.06×10^{-4}	1.97×10^{-4}
[t, t+2000 yr]	5.82×10^{-3}	5.68×10^{-3}	1.22×10^{-2}	3.95×10^{-4}	4.22×10^{-4}	8.38×10^{-4}
[t, t+5000 yr]	3.47×10^{-2}	3.41×10^{-2}	7.07×10^{-2}	2.44×10^{-3}	2.49×10^{-3}	5.20×10^{-3}
[t, t+9900 yr]	1.26×10^{-1}	1.19×10^{-1}	2.31×10^{-1}	9.37×10^{-3}	9.57×10^{-3}	1.99×10^{-2}

^a Probability for scenario $S^{+-}(t, t+\Delta t)$ calculated as shown in Eq. (12), with the subscript A selected to indicate "approximate".

^b Probability for scenario $S^{+-}(t, t+\Delta t)$ calculated with Monte Carlo procedure described in Sect. 3 and a sample size of 1×10^6 , with the subscript M selected to indicate "Monte Carlo".

^c Probability for scenario $S^{+}(t, t+\Delta t)$ calculated with Monte Carlo procedure described in Sect. 3 and a sample size of 1×10^6 , with the subscript M selected to indicate "Monte Carlo".

^d An approximate 100 $(1-\alpha)\%$ confidence interval is given by $Y/n \pm x_{1-\alpha/2} \left[Y(n-Y)/n^3 \right]^{1/2}$, where Y is number of times event occurred (e.g., 24 for $S^{+-}(t, t+100)$ and $\lambda = 3.28 \times 10^{-4} \text{ yr}^{-1}$), $x_{1-\alpha/2}$ is quantile of normal distribution (e.g., 1.96 for 95% confidence interval) and n is sample size (e.g., 1×10^6 in present analysis) (Ref. 47, pp. 99-100, Method C). Thus, the 95% confidence interval for $pS_M^{+-}(t, t+100)$ with $\lambda = 3.28 \times 10^{-4} \text{ yr}^{-1}$ is $2.40 \times 10^{-5} \pm 0.96 \times 10^{-5}$.

$$S^{+-}(\Delta t) = \{x: x \text{ an element of } S_{st} \text{ for which two or more boreholes penetrate the same waste panel, with at least one of these boreholes penetrating a pressurized brine pocket, at least one borehole not penetrating a pressurized brine pocket, and the minimum time of separation between a borehole that penetrates a pressurized brine pocket and a borehole that does not penetrate a pressurized brine pocket less than } \Delta t\} \quad (50)$$

and

$$S^{+}(\Delta t) = \{x: x \text{ an element of } S_{st} \text{ for which two or more boreholes penetrate the same waste panel, with at least one borehole penetrating a pressurized brine pocket, and the minimum time of separation between a borehole that penetrates a pressurized brine pocket and any other borehole is less than } \Delta t\} \quad (51)$$

Probabilities for $S^{+-}(\Delta t)$ and $S^{+}(\Delta t)$ are shown in Table 7. As examination of Table 7 shows, the probability of scenarios involving E1E2-type scenarios decreases as the allowed time of separation between the defining boreholes decreases. Indeed, scenarios involving E1E2-type scenarios almost go away (i.e., have probabilities approaching or less than 10^{-3}) if an argument can be made that the defining intrusions must occur within 100 yr of each other.

Table 7. Comparison of Probabilities for Scenarios Involving E1E2-Type Intrusions That Occur with Fixed Separation Times for the Defining Boreholes

Separation Time Δt	$pS_M^{+-}(\Delta t)^a$ $\lambda=3.28 \times 10^{-4} \text{ yr}^{-1}$	$pS_M^{+}(\Delta t)^b$ $\lambda=3.28 \times 10^{-4} \text{ yr}^{-1}$	$pS_M^{+-}(\Delta t)$ $\lambda=8.44 \times 10^{-5} \text{ yr}^{-1}$	$pS_M^{+}(\Delta t)$ $\lambda=8.44 \times 10^{-5} \text{ yr}^{-1}$
Constant Brine Pocket Area Fraction: $fBP = 0.45075$ (Table 5)				
100 yr	5.18×10^{-3}	7.26×10^{-3}	3.39×10^{-4}	4.65×10^{-4}
500 yr	2.50×10^{-2}	3.50×10^{-2}	1.70×10^{-3}	2.39×10^{-3}
1000 yr	4.79×10^{-2}	6.62×10^{-2}	3.33×10^{-3}	4.66×10^{-3}
2000 yr	8.63×10^{-2}	1.18×10^{-1}	6.33×10^{-3}	8.84×10^{-3}
5000 yr	1.61×10^{-1}	2.14×10^{-1}	1.27×10^{-2}	1.77×10^{-2}
9900 yr	2.02×10^{-1}	2.67×10^{-1}	1.68×10^{-2}	2.34×10^{-2}
Panel-Dependent Brine Pocket Area Fractions: $fBP_i = aBP_i/aTOT_i$ (Table 5)				
100 yr	2.92×10^{-3}	6.30×10^{-3}	1.80×10^{-4}	3.99×10^{-4}
500 yr	1.41×10^{-2}	3.02×10^{-2}	9.95×10^{-4}	2.05×10^{-3}
1000 yr	2.70×10^{-2}	5.69×10^{-2}	1.89×10^{-3}	3.96×10^{-3}
2000 yr	4.92×10^{-2}	1.01×10^{-1}	3.56×10^{-3}	7.52×10^{-3}
5000 yr	9.39×10^{-2}	1.85×10^{-1}	7.22×10^{-3}	1.51×10^{-2}
9900 yr	1.19×10^{-1}	2.31×10^{-1}	9.57×10^{-3}	1.99×10^{-2}

^a Probability for scenario $S^{+-}(\Delta t)$ calculated with Monte Carlo procedure described in Sect. 3 and a sample size of 1×10^6 , with the subscript M selected to indicate "Monte Carlo".

^b Probability for scenario $S^{+}(\Delta t)$ calculated with Monte Carlo procedure described in Sect. 3 and a sample size of 1×10^6 , with the subscript M selected to indicate "Monte Carlo".

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5. Discussion and Prospectus

A Monte Carlo procedure for the construction of CCDFs for comparison with the EPA release limits for radioactive waste disposal has been illustrated. Conceptually, this procedure is a numerical (i.e., Monte Carlo) technique for integration over the probability space $\mathcal{S}_{st}$ associated with stochastic uncertainty. In terms of computational cost, the Monte Carlo procedure is competitive with a previously used procedure based on stratified sampling and produces similar results when equivalent integration problems are considered.

Both the Monte Carlo procedure and the stratified sampling procedure make use of a relatively small number of mechanistic calculations, which are then used to construct normalized releases to the accessible environment for the large number of elements of $\mathcal{S}_{st}$ that are considered in the two procedures. The advantage of the Monte Carlo procedure is that it avoids the need to explicitly define subsets of $\mathcal{S}_{st}$ (i.e., strata) and then develop closed-form formulas for the probability of these strata. Rather, $\mathcal{S}_{st}$ is covered and appropriate probabilities developed through the random sampling associated with the Monte Carlo procedure. In the example contained in this presentation, the Monte Carlo procedure allowed a better calculation of the probabilities and normalized releases associated with E1E2-type scenarios than was obtained with stratified sampling.

In future studies, it is anticipated that the Monte Carlo procedure will allow further refinements over what can be conveniently accomplished with stratified sampling, thus producing more realistic analyses. For example, (1) a distinction can be made between a single borehole that penetrates a pressurized brine pocket and single borehole that does not penetrate a pressurized brine pocket, which is important because a waste panel fills more rapidly with brine when a pressurized brine pocket is penetrated, (2) boreholes can be assumed to close after a specified period of time rather than remaining open permanently as is now done in PAs for the WIPP, (3) E1E2-type scenarios can be assumed to occur only if the necessary boreholes occur sufficiently close together in time, (4) specific flow paths through the waste based on the location of the boreholes associated with E1E2-type scenarios can be included in the analysis rather than conservatively assuming that the flow path associated with such scenarios accesses all waste in a waste panel as is currently done in PAs for the WIPP; the effects of flow paths involving more than one waste panel can also be investigated, (5) borehole permeability can be incorporated into the analysis as a stochastic uncertainty (i.e., all boreholes need not be assumed to have the same permeability as is currently done in PAs for the WIPP), (6) inventory checks on material released from waste panels can be performed to assure that releases do not exceed the available inventory, and (7) interpolation on intrusion time can be used to make more realistic use of the mechanistic calculations on which CCDF construction is ultimately based.

Procedures can also be used to make the Monte Carlo integration over $\mathcal{S}_{st}$ more efficient. For example, a possibility is to sample a disproportionate number of elements from $\mathcal{S}_{st}$ that involve two or more drilling intrusions and then probabilistically correct for this disproportionate sampling when the derived CCDF is actually constructed. Such procedures (i.e., importance sampling) allow increased resolution in the incorporation of unlikely but risk-

significant subsets of $\mathcal{S}_{st}$ into the analysis. For example, such a procedure could be used to increase the numerical accuracy with which the effects of E1E2-type scenarios are incorporated into the analysis.

Both the Monte Carlo and stratified sampling procedures described in this presentation rely on a relatively small number of mechanistic calculations, which are then extended to provide estimates of the releases associated with a large number of different elements of $\mathcal{S}_{st}$. Neither procedure would be computationally tractable if a sequence of mechanistic calculations had to be performed for every element of $\mathcal{S}_{st}$ required in the construction of the CCDF specified in the EPA release limits. The advantage of the Monte Carlo procedure is that it allows greater resolution to be built into the use of these mechanistic calculations.

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1328	6342	D.R. Anderson
1328	6342	Staff (20)

1395 6743	V.H. Slaboszewicz
1395 6743	Staff (3)
1341 6345	R.C. Lincoln
1341 6345	Staff (9)
1341 6347	D.R. Schafer
1341 6348	J.T. Holmes
1341 6348	Staff (4)
1343 6351	R.E. Thompson
1330 6352	G. Gerstner-Miller (2)
0736 6400	N.R. Ortiz
0746 6613	R.M. Cranwell
0746 6613	R.L. Iman
0746 6613	C. Leigh
0727 6622	M.S.Y. Chu
0718 6641	R.E. Luna, Acting
0899 13414	Technical Library (5)
0619 13416	Technical Publications
0100 7613-2	Document Processing for DOE/OSTI (10)
9018 8523-2	Central Technical Files