COMPUTATIONAL STRUCTURE OF A PERFORMANCE ASSESSMENT INVOLVING STOCHASTIC AND SUBJECTIVE UNCERTAINTY

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ABSTRACT

A recent performance assessment for the Waste Isolation Pilot Plant (WIPP), which is being developed by the U.S. Department of Energy for the geologic disposal of transuranic waste, is used to illustrate the computational structure of a large analysis that maintains a separation between stochastic (i.e., aleatory) and subjective (i.e., epistemic) uncertainty. In this analysis, stochastic uncertainty arises from the many possible disruptions that could occur over the 10,000 yr regulatory period that applies to the WIPP, and subjective uncertainty arises from the imprecision with which many of the quantities required in the analysis are known. Important parts of the computational structure are (1) the use of Latin hypercube sampling to incorporate the effects of subjective uncertainty, (2) the use of Monte Carlo (i.e., random) sampling to incorporate the effects of stochastic uncertainty, and (3) the efficient use of the necessarily limited number of mechanistic calculations that can be performed to support the analysis.

1 INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) is located in southeastern New Mexico and is being developed by the U.S. Department of Energy (DOE) for the geologic disposal of transuranic (TRU) waste (U.S. DOE 1990). Waste disposal will take place in panels excavated in bedded salt approximately 2000 ft below the land surface (Figure 1).

As part of the development process for the WIPP, a sequence of performance assessments (PAs) has been carried out by Sandia National Laboratories (SNL) to organize knowledge currently available about the WIPP and to provide guidance for future research and development efforts (WIPP PA 1991, 1992; Helton et al. 1993, 1995a, 1996). The structure of these PAs derives from the U.S. Environmental Protection Agency's (EPA's) regulation for the geologic disposal of radioac-

tive waste: 40 CFR 191, Subpart B: *Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* (U.S. EPA 1985, 1993). Assessing compliance with 40 CFR 191 presents an interesting analysis problem due to the need to use detailed numerical models to evaluate potential radionuclide releases from the WIPP and requirements in the regulation for a detailed representation of the effects of different types of uncertainty.

At present (June 1996), the most recent iteration of these PAs is underway and will support an application by the DOE to the EPA for the certification of the WIPP for the disposal of TRU waste. This presentation provides an overview of the computational structure being used in this PA to assess compliance with 40 CFR 191.

2 SUMMARY OF 40 CFR 191, SUBPART B

The following is the central requirement of 40 CFR 191, Subpart B, and the primary focus of this paper:

§ 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

Figure 1: Cross-sectional view of the WIPP (Fig.1-9, Vol. 1, WIPP PA 1991; see Sect. 2.2, Vol. 2, WIPP PA 1992 for detailed stratigraphy)

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, U.S. EPA 1985). Table 1 (Appendix A) of U.S. EPA 1985 specifies allowable releases (i.e., release limits) for individual radionuclides. The WIPP is intended for TRU 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, U.S. EPA 1985). Specifically, the normalized release R for transuranic waste is defined by

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

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 (C_i), L_i is the release limit (C_i) for the radionuclide i (Table 1, App. A, U.S. EPA 1985) and C is the amount of TRU waste emplaced in the repository (C_i). For the 1996 WIPP PA, $C = 4.07 \times 10^6 \text{ Ci}$.

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* (U.S. EPA 1996). There, the following elaboration of the intent of 40 CFR 191.13 appears (pp. 5242-5243, U.S. EPA 1996):

§ 194.34 Results of performance assessments.

- (a) The results of performance assessments shall be assembled into "complementary, cumulative distribution functions" (CCDFs) that represent the probability of exceeding various levels of cumulative release caused by all significant 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 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) (Figure 2), and EN3 corresponds to the distributions indicated in 194.34(b).

3 PROBABILISTIC CHARACTERIZATION OF DIFFERENT FUTURES

The entity EN1 is the outcome of the scenario development process for the WIPP and provides a probabilistic characterization of the likelihood of different futures that could occur at the WIPP over the next 10,000 yr, with the period of 10,000 yr specified in 191.13(a). When viewed formally, EN1 is defined by a probability space $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$, with the sample space $\mathcal{S}_{st}$ given by

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

Figure 2: Boundary Line and Associated CCDF Specified in 191.13(a)

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

The following guidance (p. 5242, U.S. EPA 1996)

§ 194.32 Scope of performance assessments.

- (a) Performance assessments shall consider natural processes and events, mining, deep drilling, and shallow drilling that may affect the disposal system during the regulatory time frame.
- (b) Assessments of mining effects may be limited to changes in the hydraulic conductivity of the hydrogeologic units of the disposal system from excavation mining for natural resources. Mining shall be assumed to occur with a one in 100 probability in each century of the regulatory time frame.

and an extensive review of possible disruptions at the WIPP led to drilling intrusions and potash mining being the only occurrences incorporated into the definition of $\mathcal{S}_{st}$. Specifically, the elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$ are vectors of the form

$$\mathbf{x}_{st} = [\underbrace{t_1, a_1, b_1, l_1, p_1}_{1^{\text{st}} \text{ intrusion}}, \underbrace{t_2, a_2, b_2, l_2, p_2, \dots}_{2^{\text{nd}} \text{ intrusion}}, \dots, \underbrace{t_n, a_n, b_n, l_n, p_n, t_{\min}}_{n^{\text{th}} \text{ intrusion}}] \quad (3)$$

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

In consistency with the following guidance (p. 5242, U.S. EPA 1996)

§ 194.33 Consideration of drilling events in performance assessments.

- (2) In performance assessments, drilling events shall be assumed to occur in the Delaware Basin at random intervals in time and space during the regulatory time frame.
- (3) The frequency of deep drilling shall be calculated in the following manner:
 - (i) Identify deep drilling that has occurred for each resource in the Delaware Basin over the past 100 years prior to the time at which a compliance application is prepared.
 - (ii) The total rate of deep drilling shall be the sum of the rates of deep drilling for each resource.

the drilling rate in the vicinity of the WIPP was determined to be 46.8 intrusions/km² 10⁴ yr, which leads to a rate of

$$\begin{aligned}\lambda_d &= (46.8 / \text{km}^2 \cdot 10^4 \text{ yr}) (0.6285 \text{ km}^2) \\ &= 2.94 \times 10^{-3} \text{ yr}^{-1}\end{aligned}\quad (4)$$

for intrusions into the area (0.6285 km²) marked by a berm used as part of a passive marker system (Figure 3). Further, 100 yr of active institutional control (§194.41, p. 5243, U.S. EPA 1996) and 600 yr of passive institutional control (§194.43, p. 5243, U.S. EPA 1996) lead to the following time-dependent drilling rate:

$$\begin{aligned}\lambda_d(t) &= 0 \text{ yr}^{-1} \quad 0 \leq t \leq 100 \text{ yr} \\ &= 2.94 \times 10^{-5} \text{ yr}^{-1} \quad 100 < t \leq 700 \text{ yr} \\ &= 2.94 \times 10^{-3} \text{ yr}^{-1} \quad 700 < t \leq 10000 \text{ yr}.\end{aligned}\quad (5)$$

Drilling intrusions are assumed to be equally likely to occur at each node in Figure 3. Further, the analysis uses specified probabilities for: encountering no waste (0.80), CH waste (0.18), or RH waste (0.02); encountering pressurized brine (0.08); and use of a one (0.02), two

TRI- 6342-4698-0

Figure 3: Discretized Locations for Drilling Intrusions Used in 1996 WIPP PA

(0.68) or three plug (0.30) procedure to seal boreholes. The CH waste is emplaced in the repository in 55-gallon drums that come from 569 distinct waste streams, which also have assigned probabilities. As the CH waste is emplaced in the repository in drums stacked three high, each drilling intrusion into CH waste is assumed to intersect three randomly selected waste streams. Finally, the distribution for $t_{\min}$ is defined by the assumption that potash mining occurs at a rate of $\lambda_m = 1 \times 10^{-4} \text{ yr}^{-1}$ (194.32(b)). The preceding assumptions define $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$.

4 ESTIMATION OF RELEASES

The entity EN2 is the outcome of the model development process for the WIPP and provides a way to estimate radionuclide releases to the accessible environment (i.e., values for Q_i and hence R in Eq. (1)) for the different futures (i.e., elements $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$) that could occur at the WIPP. Estimation of environmental releases corresponds to evaluation of the function f in Figure 2. Release mechanisms associated with f include direct removal to the surface at the time of a drilling intrusion (i.e., cuttings, spallings, brine flow) and release subsequent to a drilling intrusion due to brine flow up a borehole with a degraded plug (i.e., groundwater transport).

The primary computational models in the 1996 WIPP PA are illustrated in Figure 4. Most of these models involve the numerical solution of partial differential equations used to represent material deformation, fluid flow or radionuclide transport. It is the models in Figure 4 that actually define the function f in Figure 2.

As indicated in Figure 2, the CCDF specified in 191.13(a) can be formally defined by an integral of f over $\mathcal{S}_{st}$. In practice, this CCDF is never obtained by direct evaluation of an integral due to the complexity of f and $\mathcal{S}_{st}$. Rather, an approximation procedure based on importance sampling (Helton and Iuzzolino 1993, Helton 1994) or Monte Carlo (random) sampling (Helton and Shiver 1996) is used. The 1996 WIPP PA uses a Monte Carlo procedure. Specifically, elements

$$\mathbf{x}_{st,i}, i = 1, 2, \dots, nS, \quad (6)$$

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

$$\begin{aligned} \text{prob}(\text{Rel} > R) &= \int_{\mathcal{S}_{st}} \delta_R[f(\mathbf{x}_{st})] d_{st}(\mathbf{x}_{st}) dV_{st} \\ &\doteq \sum_{i=1}^{nS} \delta_R[f(\mathbf{x}_{st,i})] / nS. \end{aligned} \quad (7)$$

The models in Figure 4 are too computationally intensive to permit their evaluation for every element $\mathbf{x}_{st,i}$ of $\mathcal{S}_{st}$ in Eq. (6). Due to this constraint, the models in Figure 4 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 $\mathbf{x}_{st,i}$ in Eq. (7).

Figure 4: Computer Programs (Models) Used in 1996 WIPP PA

5. PROBABILISTIC CHARACTERIZATION OF PARAMETER UNCERTAINTY

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 $(\mathcal{S}_{su}, \mathcal{L}_{su}, p_{su})$, with the sample space $\mathcal{S}_{su}$ given by

$$\mathcal{S}_{su} = \{\mathbf{x}_{su}: \mathbf{x}_{su} \text{ is possibly the correct vector of parameter values to use in the WIPP PA}\}. \quad (8)$$

The subscript su refers to subjective (i.e., epistemic) uncertainty and is used because $(\mathcal{S}_{su}, \mathcal{L}_{su}, p_{su})$ is providing a probabilistic characterization of where the appropriate inputs to use in the WIPP PA are believed to be located. In practice, $\mathbf{x}_{su}$ is a vector of the form

$$\mathbf{x}_{su} = [x_1, x_2, \dots, x_{nV}], \quad (9)$$

where nV is the number of uncertain variables under consideration, and $(\mathcal{S}_{su}, \mathcal{L}_{su}, p_{su})$ is obtained by specifying a distribution

$$D_j, j = 1, 2, \dots, nV, \quad (10)$$

for each element x_j of $\mathbf{x}_{su}$. The preceding distributions correspond to the distributions in 194.34(b).

In concept, some elements of $\mathbf{x}_{su}$ can affect the definition of $(\mathcal{S}_{st}, \mathcal{L}_{st}, p_{st})$ (e.g., the rate constant λ_d in Eq. (4) used to define the Poisson process for drilling intrusions) and other elements relate to the models in Figure 4 that determine the function f in Figure 2 and Eq. (7) (e.g., radionuclide solubilities in Castile brine or fracture spacing in the Culebra Dolomite). However, all elements of $\mathbf{x}_{su}$ in the 1996 WIPP PA relate to the models in Figure 4 (Table 1).

If the value for $\mathbf{x}_{su}$ was precisely known, then the CCDF in Figure 2 could be determined with certainty and compared with the boundary line specified in 191.13(a). However, given the complexity of the WIPP site and the 10,000 yr period under consideration, $\mathbf{x}_{su}$ can never be known with certainty. Rather, uncertainty in $\mathbf{x}_{su}$ as characterized by $(\mathcal{S}_{su}, \mathcal{L}_{su}, p_{su})$ will lead to a distribution of CCDFs as indicated in 194.34(c) and (e) (Figure 5). The proximity of this distribution to the boundary line in Figure 2 provides an indication of the confidence that 191.13(a) will be met as required in 191.13(b).

Table 1: Four Examples of the $nV = 57$ Uncertain Input Variables (i.e., elements x_j of $\mathbf{x}_{su}$) Considered in the 1996 WIPP PA

WGRMICI: Gas generation rate due to microbial degradation of cellulose under inundated conditions. Used in BRAGFLO. Range: 3.17×10^{-10} to 9.51×10^{-9} mol/kg-cellulose. Distribution: Uniform.

BHPERM: Borehole permeability. Used in BRAGFLO. Range: 1×10^{-14} to 1×10^{-11} m². Distribution: Loguniform.

WTAUFAIL: Shear strength of waste. Used in CUTTINGS. Range: 0.05 to 10 Pa. Distribution: Uniform.

CKDPU3: Distribution coefficient for plutonium in the +3 oxidation state in the Culebra Dolomite. Used in SECO-TRANSPORT. Range: 0.02 to 0.5 m³/kg. Distribution: Uniform.

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Figure 5. Distribution of CCDFs Resulting from Possible Values for $\mathbf{x}_{su} \in \mathcal{S}_{su}$

The distribution of CCDFs in Figure 5 can be summarized by distributions of exceedance probabilities conditional on individual release values (Figure 6). Specifically, Figure 6 shows the distribution of exceedance probabilities associated with the release of size R indicated in Figure 5. In concept, this distribution is defined

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Figure 6: Distribution of Exceedance Probabilities for a Normalized Release of Size R (Figure 5) Due to Subjective Uncertainty

by a double integral over $\mathcal{S}_{su}$ and $\mathcal{S}_{st}$. In practice, this integral is too complex to permit a closed-form evaluation. Instead, the 1996 WIPP PA uses Latin hypercube sampling (McKay et al. 1979) to evaluate the integral over $\mathcal{S}_{su}$ and, as indicated in Eq. (7), simple random sampling to evaluate the integral over $\mathcal{S}_{st}$.

Specifically, a Latin hypercube sample (LHS)

$$\mathbf{x}_{su,k}, k = 1, 2, \dots, nLHS, \quad (11)$$

is generated from $\mathcal{S}_{su}$ in consistency with the definition of $(\mathcal{S}_{su}, \mathcal{J}_{su}, p_{su})$ and a random sample as indicated in Eq. (6) is generated from $\mathcal{S}_{st}$ in consistency with the definition of $(\mathcal{S}_{st}, \mathcal{J}_{st}, p_{st})$. The percentile values in Figure 6 (i.e., $P_{0.1}$, $P_{0.5}$, $P_{0.9}$) are then approximated by solving

$$prob(p \leq P | R) \doteq 1 - \sum_{k=1}^{nLHS} \delta_P \left[\sum_{i=1}^{nS} \delta_R [f(\mathbf{x}_{st,i}, \mathbf{x}_{su,k})] / nS \right] / nLHS \quad (12)$$

for P with $\text{prob}(p \leq P|R) = 0.1, 0.5$ and 0.9 , respectively. Similarly, the mean exceedance probability $\bar{P}$ is approximated by

$$\bar{P} \doteq \sum_{k=1}^{nLHS} \left[\sum_{i=1}^{nS} \delta_R[f(\mathbf{x}_{st,i}, \mathbf{x}_{su,k})] / nS \right] / nLHS. \quad (13)$$

The results of the preceding calculations are typically displayed by plotting percentile values (e.g., $P_{0.1}$, $P_{0.5}$, $P_{0.9}$) and also the mean values (i.e., $\bar{P}$) for the exceedance probabilities above individual release values (i.e., R) and then connecting these points to form continuous curves (Figure 7). The proximity of these curves to the boundary line provides an indication of the confidence with which 191.13(a) will be met.

6. COMPUTATIONAL DETAILS OF 1996 WIPP PA

The requirements in 194.34(c), (d) and (f) interact in determining the details of the 1996 WIPP PA. Requirements 194.34(c) and (d) can be satisfied with a random sample from S_{su} of size 298 (i.e., $1 - 0.99^n > 0.95$ yields $n = 298$). However, the WIPP PA decided to use Latin hypercube sampling because of the efficient manner in which it stratifies across the range of each uncertain parameter (Iman and Helton 1988) and the observed stability of uncertainty and sensitivity analysis results produced in past analyses that involved a separation of stochastic and subjective uncertainty (Iman and Helton 1991, Helton et al. 1995b).

Given that Latin hypercube sampling is to be used, the confidence intervals required in 194.34(f) can be obtained with a replicated sampling technique proposed by R.L. Iman (1982). In this technique, the LHS in Eq. (11) is repeatedly generated with different random seeds. These samples lead to a sequence $\bar{P}_r(R)$, $r = 1, 2, \dots, nR$, of estimated mean exceedance probabilities, where $\bar{P}_r(R)$ defines the mean CCDF obtained for sample r (i.e., $\bar{P}_r(R)$ is the mean probability that a normalized release of size R will be exceeded) and nR is the number of independent LHSs generated with different random seeds. Then,

$$\bar{P}(R) = \sum_{r=1}^{nR} \bar{P}_r(R) / nR \quad (14)$$

and

$$SE(R) = \left\{ \sum_{r=1}^{nR} [\bar{P}_r(R) - \bar{P}(R)]^2 / nR(nR - 1) \right\}^{1/2} \quad (15)$$

provide an additional estimate of the mean CCDF and an estimate of the standard error associated with the mean exceedance probabilities. The t -distribution with $nR-1$ degrees of freedom can be used to place confidence intervals around the mean exceedance probabilities for individual R values (i.e., around $\bar{P}(R)$). Specifically, the $1-\alpha$ confidence interval is given by $\bar{P}(R) \pm t_{1-\alpha/2} SE(R)$, where $t_{1-\alpha/2}$ is the $1-\alpha/2$ quantile of the t -distribution with $nR-1$ degrees of freedom (e.g., $t_{1-\alpha/2} = 4.303$ for $\alpha = 0.05$ and $nR = 3$). The same procedure can also be used to place pointwise confidence intervals around percentile curves.

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Figure 7: Example CCDF Distribution from 1992 WIPP PA (WIPP PA 1992)

To implement the preceding procedure, the 1996 WIPP PA is using $nR = 3$ replicated LHSs of size $nLHS = 100$ each (see Eq. (11)). This produces a total of 300 observations, which is approximately the same as the sample size of 298 indicated above. Each sample is generated with the restricted pairing technique developed by Iman and Conover (1982) to induce specified rank correlations between correlated variables and also to assure that uncorrelated variables have correlations close to zero.

Once the indicated LHSs are generated, calculations are performed with the models in Figure 4 for the individual sample elements. The number of individual model calculations is too large to describe here. However, the basic strategy is to avoid the unnecessary proliferation of computationally demanding calculations by identifying situations where (1) a single computationally demanding calculation can be used to supply input to several less demanding calculations, (2) mathematical properties of the models can be used to extend the results of a single calculation to many different situations, or (3) a relatively inexpensive screening calculation can be used to determine if a more detailed, and hence more expensive, calculation is needed. As examples, (1) each BRAGFLO calculation, which involves the numerical solution of a system of nonlinear partial differential equations and is quite demanding computationally (i.e., 1 - 2 hrs of CPU time on a Digital VAX Alpha using VMS), is used to supply conditions that are used in a number of different calculations with the SPALLINGS, BRINEFLO, NUTS and PANEL models indicated in Figure 4; (2) the linearity of the system of partial differential equations that underlies SECO-TRANSPORT makes it possible to perform transport calculations for unit releases of individual radionuclides to the Culebra Dolomite and then use the outcome of these calculations to construct transport results for arbitrary time-dependent radionuclide releases into the Culebra; and (3) transport calculations with NUTS are initially performed with a nondecaying tracer and then calculations with radionuclides are only performed for those cases that have a potential to result in a radionuclide release from the repository.

The analysis effort for all three replications was still quite large and involved 1800 BRAGFLO calculations, 15,600 CUTTINGS/SPALLINGS calculations (Note: What is designated as CUTTINGS and SPALLINGS in Figure 4 is actually a single program), 15,600 BRINEFLO calculations (Note: BRINEFLO is actually a special configuration of BRAGFLO used to estimate brine releases, i.e., blowout, at the time of a drilling intrusion), approximately 1500 screening and 500 full calculations with NUTS, 2100 PANEL calculations, 100 GRASP_INV calculations, 600 SECO-FLOW calculations, and 1200 SECO-TRANSPORT calculations. The

outcome of these calculations is a set of results for each LHS element.

As discussed in conjunction with Eq. (7), Monte Carlo procedures are then used to construct a CCDF for each LHS element. Specifically, this CCDF is produced from $nS = 10,000$ randomly selected futures of the form shown in Eq. (3), where nS is the sample size in Eq. (6). Once each future $\mathbf{x}_{st,i}$ is sampled, the corresponding normalized release $f(\mathbf{x}_{st,i})$ is constructed from releases to the accessible environment calculated with CUTTINGS, SPALLINGS, BRINEFLO, NUTS and SECO-TRANSPORT. In this procedure, extensive algebraic manipulations and interpolations are performed to estimate releases for futures involving multiple intrusions from the results of the previously indicated calculations for one or two intrusions at fixed points in time. Once values for $f(\mathbf{x}_{st,i})$ are determined, which correspond to the normalized release R in Eq. (1), the CCDF specified in 191.13(a) is readily constructed.

Repetition of the preceding procedure for each LHS element yields a distribution of CCDFs of the form in Figure 7 for each of the $nR = 3$ replicates as requested in 194.34(e). Further, the replicated samples and the procedure in Eqs. (14) and (15) provide a basis for the estimation of confidence intervals as requested in 194.34(f).

To this point, the emphasis of this presentation has been on uncertainty analysis. However, the techniques in use also provide a basis for sensitivity analysis. Specifically, Latin hypercube sampling generates a mapping from analysis input (i.e., elements $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$) to analysis results that can be explored with sensitivity analysis techniques based on examination of scatterplots, correlation analysis, regression analysis, and other procedures for investigating multivariate data (Helton 1993). Quantities that can be investigated include both the results from individual models and the final CCDFs. Sensitivity analysis plays three important roles by (1) identifying the effects of individual variables (i.e., elements x_j of $\mathbf{x}_{su}$), (2) providing programmatic direction as to where resources can be invested to reduce the uncertainty in analysis outcomes, and (3) facilitating quality assurance by systematically examining the effects of many combinations of analysis inputs on a variety of analysis results. Sensitivity analysis procedures will be used extensively to study the outcomes of the 1996 WIPP PA.

7 STATUS

The calculations described in this presentation are currently underway at SNL and are anticipated to be completed by the end of July 1996. Extensive documentation of these calculations will be published by SNL and the DOE.

REFERENCES

- Helton, J.C. 1993. Uncertainty and Sensitivity Analysis Techniques for Use in Performance Assessment for Radioactive Waste Disposal. *Reliability Engineering and System Safety* 42: 327-367.
- Helton, J.C. 1994. Treatment of Uncertainty in Performance Assessments for Complex Systems. *Risk Analysis* 14: 483-511.
- Helton, J.C., and H.J. Iuzzolino. 1993. Construction of Complementary Cumulative Distribution Functions for Comparison with the EPA Release Limits for Radioactive Waste Disposal. *Reliability Engineering and System Safety* 40: 277-293.
- Helton, J.C., and A.W. Shiver. 1996. A Monte Carlo Procedure for the Construction of Complementary Cumulative Distribution Functions for Comparison with the EPA Release Limits for Radioactive Waste Disposal. *Risk Analysis* 16: 43-55.
- Helton, J.C., et al. 1993. Uncertainty and Sensitivity Analysis Results Obtained in a Preliminary Performance Assessment for the Waste Isolation Pilot Plant. *Nuclear Science and Engineering* 114: 286-331.
- Helton, J.C., et al. 1995a. Effect of Alternative Conceptual Models in a Preliminary Performance Assessment for the Waste Isolation Pilot Plant. *Nuclear Engineering and Design* 154: 251-344.
- Helton, J.C., et al. 1995b. Robustness of an Uncertainty and Sensitivity Analysis of Early Exposure Results with the MACCS Reactor Accident Consequence Model. *Reliability Engineering and System Safety* 48: 129-148.
- Helton, J.C., et al. 1996. Uncertainty and Sensitivity Analysis Results Obtained in the 1992 Performance Assessment for the Waste Isolation Pilot Plant. *Reliability Engineering and System Safety* 51: 53-100.
- Iman, R.L. 1982. Statistical Methods for Including Uncertainties Associated with Geologic Isolation of Radioactive Waste Which Allow for a Comparison with Licensing Criteria. *Proceedings of the Symposium on Uncertainties Associated with the Regulation of the Geologic Disposal of High Level Radioactive Waste*, Gatlinburg, Tennessee, March 9-13, 1981, ed. D.C. Kocher. NUREG/CP-0022, CONF-810372. Oak Ridge National Laboratory, Oak Ridge, Tennessee, 145-157.
- Iman, R.L., and W.J. Conover. 1982. A Distribution-Free Approach to Inducing Rank Correlation Among Input Variables. *Communications in Statistics B11*: 311-334.
- Iman, R.L., and J.C. Helton. 1988. An Investigation of Uncertainty and Sensitivity Analysis Techniques for Computer Models. *Risk Analysis* 8: 71-90.
- Iman, R.L., and J.C. Helton. 1991. The Repeatability of Uncertainty and Sensitivity Analyses for Complex Probabilistic Risk Assessments. *Risk Analysis* 11: 591-606.
- McKay, M.D., W.J. Conover, and R. J. Beckman. 1979. A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code. *Technometrics* 21: 239-245.
- U.S. DOE (Department of Energy). 1990. *Final Supplement Environmental Impact Statement, Waste Isolation Pilot Plant*. DOE/EIS-0026-FS. U.S. Department of Energy, Office of Environmental Restoration and Waste Management, Washington, DC.
- U.S. EPA (Environmental Protection Agency). 1985. Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Waste; Final Rule, 40 CFR Part 191. *Federal Register* 50: 38066-38089.
- U.S. EPA (Environmental Protection Agency). 1993. Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Waste; Final Rule, 40 CFR Part 191. *Federal Register* 58: 66398-66416.
- U.S. EPA (Environmental Protection Agency). 1996. 40 CFR Part 194: Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance With the 40 CFR Part 191 Disposal Regulations; Final Rule. *Federal Register* 61: 5224-5245.
- WIPP PA (Performance Assessment) Division. 1991. *Preliminary Comparison with 40 CFR Part 191, Subpart B for the Waste Isolation Pilot Plant, December 1991*, Vols. 1-4. SAND91-0893/1-4. Sandia National Laboratories, Albuquerque, New Mexico.
- WIPP PA (Performance Assessment) Department. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992*, Vols. 1-5. SAND92-0700/1-5. Sandia National Laboratories, Albuquerque, New Mexico.

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