Uncertainty Analysis in the 1996 Performance Assessment for the Waste Isolation Pilot Plant

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1 Introduction

The appropriate treatment of uncertainty is now widely recognized as an essential component of performance assessments (PAs) for complex systems.[1-3] When viewed at a high-level, the uncertainty in such analyses can typically be partitioned into two types: (i) stochastic uncertainty, which arises because the system can behave in many different ways and is thus a property of the system itself, and (ii) subjective uncertainty, which arises from a lack of knowledge about quantities that are believed to have (or, at least, are assumed to have) fixed values and is thus a property of the analysts carrying out the study.[4,5] Alternative names include aleatory, type A, irreducible and variability as substitutes for the designation stochastic, and epistemic, type B, reducible and state of knowledge as substitutes for the designation subjective. The treatment of uncertainty in these two contexts can be traced back to the beginnings of the formal development of the theory of probability.[6]

The 1996 PA for the Waste Isolation Pilot Plant (WIPP) carried out at Sandia National Laboratories (SNL) will be used to illustrate the treatment of these two types of uncertainty in a real analysis.[7] In particular, this PA supported a compliance certification application (CCA) by the U.S. Department of Energy (DOE) to the U.S. Environmental Protection Agency (EPA) for the certification of the WIPP for the geologic disposal of transuranic waste.[8] A similar structure was also used in the U.S. Nuclear Regulatory Commission's (NRC's) reassessment of the Reactor Safety Study (NUREG-1150) but in the context of probabilistic risk assessments (PRAs) for nuclear power stations.[9,10] Insights on the conceptual and computational structure of PAs for complex systems gained from these and other analyses are being incorporated into a new software system under development at SNL to facilitate the performance of analyses that maintain a separation between stochastic and subjective uncertainty.

2 Stochastic Uncertainty in the 1996 WIPP PA

Stochastic uncertainty enters the 1996 WIPP PA due to the different disruptions that could occur at the WIPP over the 10,000 yr regulatory period specified in the

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EPA's regulations for the disposal of radioactive waste.[11,12] The WIPP PA uses probability to characterize stochastic uncertainty. In particular, a probability space $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ for stochastic uncertainty is introduced. The elements $\mathbf{x}_{st}$ of the sample space $\mathcal{S}_{st}$ are vectors characterizing sequences of random events that could occur at the WIPP over the next 10,000 yr and have the form

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

where n is the number of drilling intrusions in the vicinity of the WIPP, t_i is the time (yr) of the ith intrusion, l_i designates the location of the ith intrusion, e_i designates the penetration of an excavated or nonexcavated area by the ith intrusion, b_i designates whether or not the ith intrusion penetrates pressurized brine in the Castile Formation, p_i designates the plugging procedure used with the ith intrusion (i.e., continuous plug, two discrete plugs, three discrete plugs), $\mathbf{a}_i$ designates the type of waste penetrated by the ith intrusion (i.e., no waste, contact-handled (CH) waste, remotely-handled (RH) waste), and t_{min} is the time at which potash mining occurs within the land withdrawal boundary. Specification of distributions for the elements of $\mathbf{x}_{st}$ then leads to a definition for $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ (Ref. 13; Chapt. 3, Ref. 7).

Each future $\mathbf{x}_{st}$ leads to a normalized release to the accessible environment, which can be represented by a function $f(\mathbf{x}_{st})$ (Ref. 13; Chapt. 4, Ref. 7). The EPA's regulations[11,12] require that the information associated with $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ and f be summarized by a complementary cumulative distribution function (CCDF) (Fig. 1). In turn, the exceedance probabilities associated with this CCDF can be formally represented by the integral

$$prob(Rel > R) = \int_{\mathcal{S}_{st}} \delta_R[f(\mathbf{x}_{st})] d_{st}(\mathbf{x}_{st}) dV_{st}, \quad (2)$$

where $\delta_R[f(\mathbf{x}_{st})] = 1$ if $f(\mathbf{x}_{st}) > R$ and 0 if $f(\mathbf{x}_{st}) \leq R$, $d_{st}(\mathbf{x}_{st})$ is the density function associated with $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$, and the differential dV_{st} is used because $\mathcal{S}_{st}$ is multidimensional (see Fig. 1, Ref. 13).

Evaluating the preceding integral, or at least determining an approximation to it, is a major undertaking as both $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ and f are quite complex in the 1996 WIPP PA. Earlier PAs for the WIPP used an importance sampling procedure to evaluate this integral.[14] However, the 1996 WIPP PA used a Monte Carlo procedure,[15] with the approximation having the form

$$prob(Rel > R) \doteq \sum_{i=1}^{nS} \delta_R[f(\mathbf{x}_{st,i})] / nS, \quad (3)$$

where $\mathbf{x}_{st,i}$, $i = 1, 2, \dots, nS$, is a random sample obtained in consistency with the definition of $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ (Sect. 6.6, Ref. 7) and a rather elaborate numerical
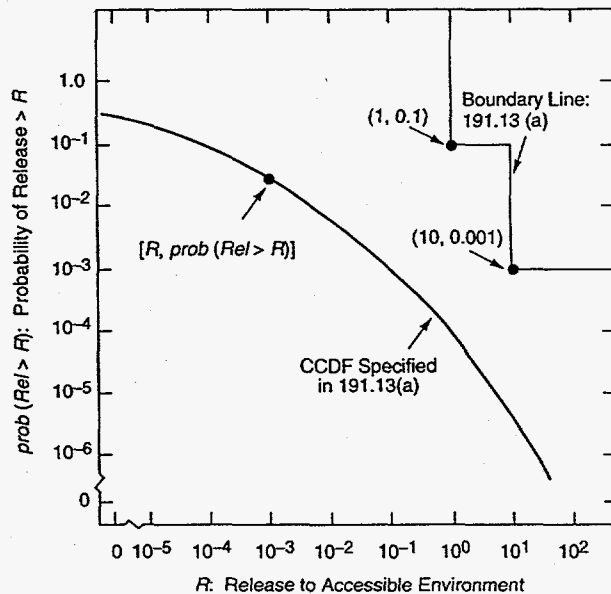
Fig. 1. Boundary line and associated CCDF specified in 40 CFR 191, Subpart B (Refs. 11, 12).

procedure is used to obtain values for $f(\mathbf{x}_{st,i})$. In particular, a limited number of mechanistic calculations were performed for selected elements of S_{st}, and then the results of these calculations were used to construct the required values of $f(\mathbf{x}_{st,i})$ in Eq. (3). In contrast, the NUREG-1150 PRAs performed conceptually equivalent integral evaluations with an importance sampling procedure based on the use of event trees to decompose the sample space associated with stochastic uncertainty.

3 Subjective Uncertainty in the 1996 WIPP PA

Subjective uncertainty enters the 1996 WIPP PA due to a lack of knowledge with respect to the appropriate values to use for many of the parameters required in the computational implementation of this analysis. As for stochastic uncertainty, the WIPP PA uses probability to characterize subjective uncertainty. In particular, a probability space $(S_{su}, \mathcal{A}_{su}, p_{su})$ for subjective uncertainty is introduced. The elements $\mathbf{x}_{su}$ of the sample space S_{su} are vectors whose elements are imprecisely-known inputs to the analysis and have the form

$$\mathbf{x}_{su} = [x_1, x_2, ..., x_{nV}], \tag{4}$$

where each $x_j, j = 1, 2, ..., nV$, is an imprecisely-known input (e.g., inputs related to permeabilities, gas generation rates, solubilities, retardations, ...; see App. PAR, Ref. 8, and Table 5.2.1, Ref. 7, for a complete listing of the $nV = 57$ elements of $\mathbf{x}_{su}$ and sources of additional information).

The effects of subjective uncertainty are typically presented in one of two ways: (i) a distribution over subjective uncertainty conditional on a fixed element $\mathbf{x}_{st}$ of $\mathcal{S}_{st}$, and (ii) a distribution of CCDFs over subjective uncertainty, with each CCDF arising from stochastic uncertainty and conditional on a fixed element $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$. In the first case, the distribution can be formally expressed as

$$prob(Rel > R|\mathbf{x}_{st}) = \int_{\mathcal{S}_{su}} \delta_R[f(\mathbf{x}_{st},\mathbf{x}_{su})]d_{su}(\mathbf{x}_{su})dV_{su}, \tag{5}$$

where $d_{su}(\mathbf{x}_{su})$ is the density function associated with $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ and other notation is the same as in Eq. (2). The preceding representation results in the distribution being displayed as a CCDF (Fig. 1), although other representations such as cumulative distribution functions and density functions are also possible. In a large analysis such as the 1996 WIPP PA, $f(\mathbf{x}_{st}, \mathbf{x}_{su})$ is actually vector-valued, with many thousands of components and each of these components having the potential to be represented as indicated in Eqs. (2) and (5); further, many analysis outcomes are spatially or temporally variable, which results in more complex representations (e.g., distributions of time-dependent results). As an example, Fig. 2a shows an approximation to the distribution of repository pressure conditional on the element of $\mathcal{S}_{st}$ that corresponds to undisturbed conditions.

In the second case, the integral representation for each CCDF in the distribution is

$$prob(Rel > R|\mathbf{x}_{su}) = \int_{\mathcal{S}_{st}} \delta_R[f(\mathbf{x}_{st},\mathbf{x}_{su})]d_{st}(\mathbf{x}_{st}|\mathbf{x}_{su})dV_{st}, \tag{6}$$

with the individual CCDFs arising from stochastic uncertainty and also conditional on individual elements $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$ (Fig. 2a, Ref. 13). In general, $\mathbf{x}_{su}$ can affect both
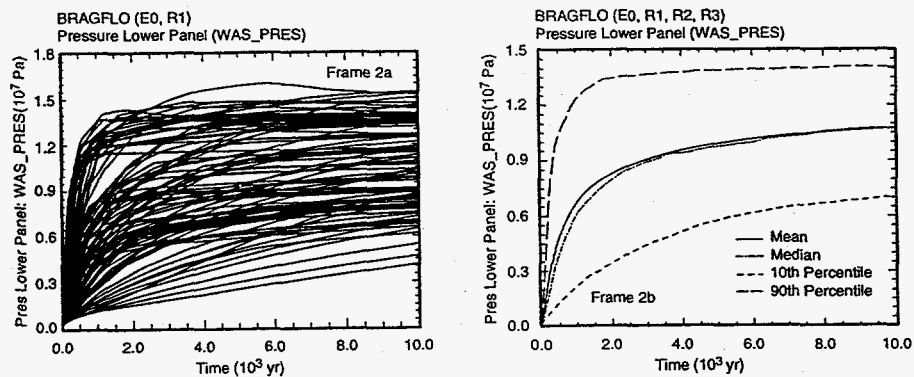
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Fig. 2. Repository pressure under undisturbed conditions: (2a) Pressure curves conditional on elements $\mathbf{x}_{su}$ of $\mathcal{S}_{su}$, and (2b) mean and percentile curves obtained by integrating over $\mathcal{S}_{su}$.

f and $(S_{st}, \mathcal{A}_{st}, p_{st})$, although in the 1996 WIPP PA all components of $\mathbf{x}_{su}$ were used in the evaluation of f.

Determination of the effects of subjective uncertainty corresponds to the evaluation of integrals involving the probability space $(S_{su}, \mathcal{A}_{su}, p_{su})$. For example, the mean curve in Fig. 2b is defined by

$$\overline{pres}(t|\mathbf{x}_{st}) = \int_{S_{su}} f(\mathbf{x}_{st}, \mathbf{x}_{su}, t) d_{su}(\mathbf{x}_{su}) dV_{su}, \tag{7}$$

where $\overline{pres}(t|\mathbf{x}_{st})$ is the mean pressure in the repository at time t given element $\mathbf{x}_{st}$ of S_{st} and $f(\mathbf{x}_{st}, \mathbf{x}_{su}, t)$ corresponds to the pressure at time t obtained with elements $\mathbf{x}_{st}$ and $\mathbf{x}_{su}$ of S_{st} and S_{su}, respectively. Similarly, the mean curve in Fig. 2b of Ref. 13 is defined by

$$\overline{prob}(Rel > R) = \int_{S_{su}} \left[\int_{S_{st}} \delta_R[f(\mathbf{x}_{st}, \mathbf{x}_{su})] d_{st}(\mathbf{x}_{st}|\mathbf{x}_{su}) dV_{st} \right] d_{su}(\mathbf{x}_{su}) dV_{su}, \tag{8}$$

where $\overline{prob}(Rel > R)$ is the mean probability over subjective uncertainty that a release (or some other analysis outcome of interest defined by f) of size R will be exceeded. The quantile curves in the indicated figures are defined by similar, but somewhat more complicated, integrals.[16]

In practice, the integrals over S_{su} indicated in Eqs. (7) and (8) are too complex to be evaluated with a closed-form procedure. Instead, some type of approximation must be used. The 1996 WIPP PA used Latin hypercube sampling to approximate integrals over S_{su}. In particular, a Latin hypercube sample (LHS) $\mathbf{x}_{su,k}$, $k = 1, 2,$ ..., $nLHS$, of size $nLHS$ was generated from S_{su} in consistency with the distributions that define $(S_{su}, \mathcal{A}_{su}, p_{su})$. Then, the results in Eqs. (7) and (8) were approximated by

$$\overline{pres}(t|\mathbf{x}_{st}) \doteq \sum_{k=1}^{nLHS} f(\mathbf{x}_{st}, \mathbf{x}_{su,k}, t) / nLHS \tag{9}$$

and

$$\overline{prob}(Rel > R) \doteq \sum_{k=1}^{nLHS} \left[\sum_{i=1}^{nS} \delta_R[f(\mathbf{x}_{st,i}, \mathbf{x}_{su,k})] / nS \right] / nLHS, \tag{10}$$

respectively, where the $\mathbf{x}_{st,i}$ are the elements of the sample used in Eq. (3). Similar approximations lead to the quantile curves in Fig. 2b and Fig. 2b of Ref. 13.

The individual curves in Fig. 2a and Fig. 2a of Ref. 13 were obtained from the indicated LHS. Although not emphasized in this presentation, these curves and other similar results constitute a mapping from uncertain analysis inputs to uncertain analysis results that can be explored with regression-based sensitivity

analysis procedures.[7,17] The NUREG-1150 PRAs also used Latin hypercube sampling to integrate over subjective uncertainty.

4 Future Developments

At present (April 1998), it is anticipated that the WIPP will be certified to begin operation before the end of 1998.[13] However, once the WIPP begins operation, a PA to support required recertifications will have to be carried out every five years.[12] To facilitate these PAs, work is currently underway at SNL to develop a software system to help automate this work to the extent practicable. Further, the system is being developed to be quite general with respect to the PA problems that it can be applied to. To this end, the system is being developed so that it can be applied to problems that can be abstracted into the three basic entities used in the preceding description of the 1996 WIPP PA: (i) a probabilistic characterization of stochastic uncertainty (i.e., $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$), (ii) a probabilistic characterization of subjective uncertainty (i.e., $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$), and (iii) a function that determines consequences of interest (i.e., $f(\mathbf{x}_{st}, \mathbf{x}_{su})$). In practice, $(\mathcal{S}_{st}, \mathcal{A}_{st}, p_{st})$ and $(\mathcal{S}_{su}, \mathcal{A}_{su}, p_{su})$ will be defined by distributions assigned to the individual components of the elements $\mathbf{x}_{st}$ and $\mathbf{x}_{su}$ of $\mathcal{S}_{st}$ and $\mathcal{S}_{su}$, and f will be defined by a user-supplied function. Further, the system will provide several options for the evaluation of the integrals indicated in this presentation, including random sampling, Latin hypercube sampling and importance sampling.

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