SAND 2003-4366J

Assignment of Probability Distributions for Parameters in the 1996 Performance Assessment for the Waste Isolation Pilot Plant Part 1: Description of Process

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Abstract

A managed process was used to consistently and traceably develop probability distributions for parameters representing epistemic uncertainty in four preliminary and the final 1996 performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The key to the success of the process was the use of a three-member team consisting of a Parameter Task Leader, PA Analyst, and Subject Matter Expert. This team, in turn, relied upon a series of guidelines for selecting distribution types. The primary function of the guidelines was not to constrain the actual process of developing a parameter distribution but rather to establish a series of well-defined steps where recognized methods would be consistently applied to all parameters. An important guideline was to use a small set of distributions satisfying the maximum entropy formalism. Another important guideline was the consistent use of the log transform for parameters with large ranges (i.e., maximum/minimum > 10^3). A parameter development team assigned 67 probability density functions (PDFs) in the 1989 PA and 236 PDFs in the 1996 PA using these and other guidelines described.

Keywords: probability distributions, maximum entropy formalism, uncertainty, risk assessment, probabilistic risk assessment, performance assessment, Monte Carlo simulations, radioactive waste disposal, nuclear waste repository, Waste Isolation Pilot Plant, 40 CFR 191, 40 CFR 197

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1. Introduction

In 1973, the citizens of Carlsbad and Eddy County in southeastern New Mexico invited the Atomic Energy Commission (AEC), forerunner to the U.S. Department of Energy (DOE), to explore the salt beds in the Delaware Basin for disposal of radioactive waste. By 1976, a suitable site had been found for more detailed characterization. This site became the Waste Isolation Pilot Plant (WIPP), a repository for disposal of transuranic (TRU) waste that was certified by the U.S. Environmental Protection Agency (EPA) in 1998 (Fig. 1). Technical results from a performance assessment (PA) conducted by Sandia National Laboratories and described in the Compliance Certification Application (CCA), submitted in October 1996 [1; 4; 5; 6], was a key component to EPA's decision to certify WIPP.

Many natural and political aspects of the project made it possible to certify the WIPP. For instance, the bedded salt of the Salado Formation (Fm) (hereafter "Salado") has excellent properties for isolating radioactive waste (thickness, purity, no evidence of dissolution, and tectonic stability); the overlying strata such as the Culebra Dolomite Member of the Rustler Fm (hereafter "Culebra") contain brine not suitable for drinking without extensive treatment (Fig. 2); low population density and absence of land use conflicts, and the public in southern New Mexico supports the location of the site. The manner in which Sandia conducted the PA helped generate favorable scientific and regulatory support [7] and sustained public support for the constructed repository (Fig. 2). Much of the PA was discussed in a special issue of *Reliability Engineering & System Safety* [8] that included an article with a brief explanation of assigning the probability distributions [9] for the model parameters.[1] However, out of necessity, much detail was omitted from the article. The same is true for earlier reports [e.g., 5; 11; 12; 13; 14; 15],

Because the authors have frequently received questions on the many issues of parameter choice that presented themselves, and because the important task of assigning distributions continues to be reported in the literature [16], this paper elaborates upon the techniques used to assign distributions for parameters in major subsystem models of the WIPP PAs. A companion paper [17] discusses the application of these techniques in assigning distributions for 24 parameters used in the WIPP PAs.

The assignment of distributions was imbedded in an overarching strategy that included iterating the PA process that is briefly described in Section 2. Although the assignment of distributions was one of the most important parts of the PA uncertainty/sensitivity analysis, in general, a complicated and elaborate process for developing distributions was judged unnecessary since the PAs were iterated. Early iterations used quickly developed, crude distributions; and later iterations, more carefully developed, refined distributions. As described in Section 3, the process involved using a team of at least three individuals who ensured understanding of (a) data available, (b) use of a parameter in the model, and (c) best practices for developing distributions. The overall process of developing distributions, presented in Section 4, consisted of a series of general steps to provide consistency in developing distributions. As described in Section 5, simple concepts from the maximum entropy formalism (MEF) [11; 18; 19]

[1] Herein, a parameter is any number or symbol that must be set by an analyst to produce meaningful output from a computationally implemented mathematical model. All model parameters may be regarded without loss of generality as elements of a set $\mathbf{p} = \{\varphi_1,.., \varphi_n,..,\varphi_{nP}\}$. Occasionally $\mathbf{p}$ is called a vector of parameters similar to the spatial vector $\mathbf{x}$. However, the parameter set $\mathbf{p}$ is not, technically speaking, a vector space [10]; hence, the use of the word "vector" for $\mathbf{p}$ can be misleading

and general recommendations gleaned from the civil engineering, policy analysis, and risk literature [20; 21] were adopted in assigning distributions. A similar approach had been suggested for other radioactive waste disposal programs [22; 23; 24]. A comparison with other methods is described in Section 6.

2. Background on Overall Strategy for WIPP PAs

A performance assessment is an assessment of whether a system meets a set of performance criteria [25; 26]. As discussed more thoroughly elsewhere (e.g., Refs. [25; 27], "performance assessment" (or "PA") is a type of risk analysis [21] of what can go wrong with a geologic disposal system such as WIPP. Because data on the frequency and consequences of degradation of a never before built geologic disposal system are obviously unavailable, extrapolation of failure data to extremes is not possible. Rather, a mathematical model is built to assess the behavior of a disposal system under a set of stylized conditions to illustrate possible "futures." In the United States, uncertainty in the results of a simulation for regulatory evaluation of WIPP must also be calculated and compared to a risk-based, probabilistic performance criterion in EPA's *Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes* [28; 29; 30], 40 CFR 191, and the implementing regulation [31], 40 CFR 194. Specifically, the quantitative portion of the EPA Standard is expressed as a piecewise-uniform, complementary cumulative distribution function [CCDF] that the results from a PA are not to exceed [2; 26; 31]. Even though great expense and effort were made to improve the state of scientific and technological knowledge about the exposure pathways through the WIPP disposal system, much remained uncertain at the time of certification. For example, characteristics of the geologic barrier could only be inferred, because many of the parameters that were assigned in the mathematical model of the geologic barrier were uncertain. Three general aspects of the overall PA strategy were pertinent to the process defining the parameter uncertainty: evaluation of reasonable expectation, periodic iterations, and detailed modeling. Each aspect is described as follows.

2.1 Evaluation of Reasonable Expectation

Based on comments made by EPA's Scientific Advisory Board (SAB) [28], the EPA incorporated the concept that[2] "performance assessments need not provide complete assurance that the requirements of 191.13(a) will be met...Instead, what is required is reasonable expectation, on the basis of the record before the implementing agency, that compliance with 191.13(a) will be achieved" [27; 28; 29; 31; 33]. Early on, the WIPP Project interpreted this as requiring that the PA use an approach that quantified uncertainties realistically and over their full range, rather than one that involved conservative point estimates or a bounding assessment. By 1996, the EPA explicitly stated this intent in the implementing regulations 40 CFR 194.34.[3] Although novel in 1985 when 40 CFR 191 was first

[2] Similarly, the NRC regulation for the Yucca Mountain repository, 10 CFR 63.303 [32] requires that "DOE must demonstrate that there is a *reasonable expectation* of compliance with this subpart before a license may be issued...[where] compliance is based upon the mean of the distribution of projected doses of DOE's performance assessment which project the performance of the Yucca Mountain disposal system for 10,000 years after disposal" (emphasis added).

[3] The EPA also explicitly stated this intent in 2001 in 40 CFR 197 (Standard for Yucca Mountain) [34]: "Characteristics of reasonable expectation include that it:...(c) Does not exclude important parameters from assessments and analyses simply because they are difficult to

promulgated [27], the importance of identifying and displaying the full range of uncertainty in an analysis to help adequately explain the results and gain useful insights is now widely acknowledged [35; 36; 37]. This approach placed a requirement to be neither too optimistic about the information that was available nor too pessimistic about the uncertainty in the data when assigning parameter values. As pointed out below, PA iterations allowed the WIPP Project to asymptotically approach this ideal rather than attempt to gain the ideal immediately.

2.2 Iterations of PA

In 1989, the WIPP PA Analysts adopted the idea of conducting sequential PAs, that is, conducting an initial PA with simple or incomplete models and preliminary data, followed by other PAs with emerging data and/or more refined models based on results of the earlier studies [2]. Prior to the PA for compliance certification conducted in 1996 [1; 5], four preliminary PAs were conducted between 1989 and 1992 [38; 39; 40; 41; 42; 43]. Currently, PA analysis continues in preparation for re-certification, which is required every five years during operation of the WIPP [30; 44]. In general, repeating the PA process allowed PA Analysts to gain an understanding about the disposal system and how best to model the system, including the value of improved models and data. An iterative process allowed PA Analysts to evaluate the importance of uncertainty in (1) the form of the models and (2) the features, events, and processes (FEPs) to include in the model (Fig. 3). Using iterations to identify which models and FEPs to expend the most effort in characterizing had been suggested earlier when developing the PA/PRA process (e.g., [45]) and used elsewhere in policy analyses [21]. The magnitude of uncertainty from model form and FEP omission can be greater (at least in early iterations while understanding of a system is still developing [21; 42; 43]) than a third type of uncertainty and topic of this paper: uncertainty in parameters of models of the disposal system.

One advantage of iterating the PA for evaluating parameter uncertainty was that early iterations could change emphasis as related to parameter development. Specifically, early iterations could be exploratory, using unbiased but wide distributions to ensure coverage of uncertainty and give adequate opportunity for the importance of a parameter to show up in sensitivity analysis, while later iterations could use unbiased, but refined, narrow distributions that properly reflected the model scale of the computational elements (or cells) in the numerical mesh. This and other changes made to the parameters in each iteration and methodologies for developing the parameters are discussed throughout this paper.

2.3 Detailed Modeling Style

The typical steps in constructing a mathematical model are conceptual model construction (i.e., pictorial/verbal models), mathematical construction, numerical implementation in a computational model, and application of the computational model (the end-product of model development) [2; 46; 47]. Herein, the purpose of the computational models is either to evaluate the consequences of radioisotope releases to the accessible environment (i.e.,

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precisely quantify to a high degree of confidence; and (d) Focuses performance assessments and analyses upon the full range of defensible and reasonable parameter distributions rather than only upon extreme physical situations and parameter values."

"consequence" models) or to evaluate the probability of various scenarios occurring (i.e., "probability" models). Unless modified, the term "model" is synonymous in this paper with the consequence computational model and designated as $R(\bullet)$ since the operations of a computation model can be viewed as the evaluation of a function that transforms a point in a N-dimensional Euclidean domain space, $\mathcal{D}_N$, to a point in a M-dimensional Euclidean range space [46, 47]. A model of a system is "complete" or "total" if the model captures all effects or phenomena of concern to the users of the model. Because of the complexity of the geologic disposal system, the total-system model for WIPP, $R(\bullet)$, was formed by linking several submodels, $\mathcal{R}_\alpha(\bullet)$, that captured specific effects or phenomenon [1; 2; 5; 46; 47].

The simplicity and practicality of running a PA simulation depends on the level of detail and complexity of the $R(\bullet)$, and its submodels, $\mathcal{R}_\alpha(\bullet)$. Starting with the 1990 PA iteration and thereafter, Sandia mainly used detailed models directly in the PA. Comments received from the EPA [39] and the WIPP Panel of the NAS on the 1989 PA demonstration encouraged Sandia to move from simplified to more detailed models. Although some may argue that mathematical models based on partial differential equations (PDEs) are too time-consuming to be used in a PA simulation where uncertainty is propagated through the analysis using Monte Carlo techniques, Sandia purposefully chose detailed models for five of the seven submodels $\mathcal{R}_\alpha(\bullet)$ of $R(\bullet)$ and sought the computational power to make detailed modeling feasible. A detailed modeling style was generally accepted in the United States because of its earlier use in the 1975 *Reactor Safety Study* [48] and its 1990 update [49]. Furthermore, by 1995, NRC policy had called for detailed modeling with unbiased parameters in probabilistic risk assessments (PRAs) and PAs [50].

The advantages of a detailed modeling approach as related to parameters were as follows [3]: A detailed modeling approach (1) reduced the need for bounding conservatism when developing simplified models and parameters; (2) allowed the WIPP Project to better understand the proper context of the parameter use and underlying data; (3) allowed the WIPP Project to tie parameter uncertainty more directly to physically measurable data (rather than force a single parameter to represent uncertainty in many different physical processes); and (4) improved transparency and traceability in that for any one submodel or component (a) the number of parameters to be developed was decreased because parameters for both a detailed process model and PA analysis model were not needed, and (b) documentation was decreased since only one model (rather than two or more at different levels of simplification) had to be described, verified, and validated under the quality assurance (QA) procedures.

Although a detailed modeling approach was used, nonetheless, many model simplifications were still required, such as using a simplified Salado stratigraphy or using two-dimensional repository with one equivalent shaft and one intrusion borehole (Fig. 3). Some of the simplifications of the WIPP disposal system were represented by a parameter [1; 3]. For example, the change in porosity of salt over time was represented by a response surface through regression analysis developed from the simulation of salt creep with a finite-element, mechanical deformation code [17; 51]; dissolved concentration results from detailed geochemical modeling were represented in the PA by distributions of solubility parameters (S_e) [17; 52], and (3) climatic change was represented as a multiplication factor on Culebra velocity field [17; 53].

2.4 Description of Parameter Space

2.4.1 Subsets of Parameter Space

The consequence model in a PA has a corresponding set of independent spatial variables ($\mathbf{x} = [x,y,z]$), a time variable (t), and ordered "nP-tuplet" of parameters, $\mathbf{p}(\mathbf{x},t) = \{\varphi_1(\mathbf{x},t),.., \varphi_n(\mathbf{x},t),..,\varphi_{nP}(\mathbf{x},t)\}$. For each choice of values for the parameters $\mathbf{p}(\mathbf{x},t)$ there is a unique applied model result for the performance measure. For the WIPP, the performance measure was the *cumulative* (integrated over 10^4 yr) release (q) of specified radioisotopes (i) across a *boundary* (surface integral) 5 km from the WIPP site normalized by EPA-specified limits (L_i) for each radioisotope. The normalization also included a waste unit factor (f_w) that depended upon the activity placed in the repository ($f_w = W_i/10^6$ Ci where W_i is the activity in curies for α-emitting TRU waste having half-lives greater than 20 yr). Hence, the performance measure evaluated by the consequence model, $\mathsf{R}(\bullet)$, was not a direct function of time and space or the total activity in the repository:

$$\mathsf{R}(\mathbf{p}) = \sum_{i}^{nI} \frac{1}{f_w L_i} \int_0^{10^4\,\mathrm{yr}} \oint_{\ell} q_i(\mathbf{x},t;\mathbf{p})\, d\ell\, dt \qquad (1)$$

Conceptually, the parameters of $\mathsf{R}(\bullet)$ may be scalar, vectors, tensors, and functions of space and time; however, for WIPP, the modeling domain was usually divided into material regions (based on, for example, geologic strata) such that the parameters were scalar and independent of $\mathbf{x}$ and t. Exceptions included porosity of the repository room (ϕ_m) (Fig. 3), which was dependent on t as the salt crept (i.e., $\phi_m = f(t)$) [17; 51], and transmissivity ($\mathfrak{T}_K$) in the Culebra [53] (Fig. 2), which was spatially dependent on $\mathbf{x}$ ($\mathfrak{T}_K = f(\mathbf{x})$).

For the WIPP, the elements of $\mathbf{p}$ were conceptually placed in three disjoint classes [2; 54]: (1) a class ($\mathbf{p}^F = \{\varphi_1,..,\varphi_n,..,\varphi_{nF}\}$) whose elements represented fixed quantities; (2) a class, designated aleatoric parameters ($\mathbf{p}^A = \{\varphi_1,..,\varphi_n,..,\varphi_{nA}\}$), whose elements, for the WIPP, represented those aspects of the disposal system assumed to have a random character (specifically, future events) for which the EPA or PA Analysts were particularly interested and for which a probability model could be constructed to estimate the probability of occurrence; and (3) remaining uncertain parameters that were designated epistemic parameters ($\mathbf{p}^E = \{\varphi_1,..,\varphi_n,..,\varphi_{nE}\}$). By far the largest class in the WIPP PA was the certain class, and the smallest, the aleatoric class.

The distinction between the two types of uncertain parameters is discussed elsewhere [54] and reviewed in Appendix I, but briefly, aleatoric parameters configured sequences of presumably random events in the future (such as human intrusions into the WIPP); they were called "aleatoric" because uncertainty of future events was deemed irreducible. Epistemic parameters, on the other hand, usually represented physical quantities that were currently imprecisely known, but in principle could be rendered more precise by further observation or experiment. Although other theoretical divisions of the class of uncertain parameters are possible, this particular distinction between the types of uncertain parameters was useful in understanding the source of uncertainty in the results, indicating how uncertainties might be better characterized (or possibly reduced) by the collection of more data [16; 36; 37; 55; 56], and in explaining the structure of the calculation as noted in the next section [9; 54; 57; 58].

2.4.2 *Design of PA Calculation*

An important goal of the PA Calculation was to construct an empirical *distribution* of $\mathsf{R}(\mathbf{p})$ (expressed as a complementary cumulative distribution function [CCDF]) for comparison with the piecewise uniform limiting CCDF specified by the EPA in 40 CFR 191 [27; 29]. Here, we provide a brief synopsis of the PA calculation to show its relationship with the two types of parameter uncertainty by defining the CCDF using the expectation operator, $\mathcal{E}[\bullet]$ [59; 60, p. 17] :

$$\wp\{\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E,\mathbf{p}^A) > R\} = \mathcal{E}[\mathcal{H}(\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E,\mathbf{p}^A)-R)] \tag{2}$$

where R is a number ≥ 0 and $\mathcal{H}(\bullet)$ is an indicator function such that $\mathcal{H}(x) = 0$ if $x \leq 0$; $\mathcal{H}(x) = 1$ if $x > 0$. The expectation of $\mathcal{H}(\mathsf{R}(\mathbf{p}^A,\mathbf{p}^E,\mathbf{p}^F)-R)$ with respect to the set of uncertain parameters $\mathbf{p}^A$ and $\mathbf{p}^E$ is

$$\mathcal{E}[\mathcal{H}(\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E,\mathbf{p}^A)-R)] = \int_{p^E}\int_{p^A} \mathcal{H}(\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E,\mathbf{p}^A)-R)\, g(\mathbf{p}^E)\, g(\mathbf{p}^A)\, d\mathbf{p}^A\, d\mathbf{p}^E \tag{3}$$

where Eq. (3) is based on the reasonable assumption that aleatoric parameters are independent of the epistemic parameters $\mathbf{p}^E$. As thoroughly described elsewhere [9; 40; 54; 57; 61; 62], Monte Carlo techniques were used to evaluate the two integrals.

The inner integration was concerned with the space of aleatoric uncertainty, $\mathbf{p}^A$, and addressed by developing scenarios.[4] That is, $\mathsf{R}(\bullet)$ was first configured to model each of a small set of discrete scenarios that represented subsets of $\mathbf{p}^A$ and denoted generically by S_j (such as the number of exploratory drilling intrusions (nD) into the repository (Fig. 3)). The results for each scenario S_j were combined with its discrete probability as calculated with a corresponding probability model $\wp\{\mathbf{p}^F,\mathbf{p}^E,S_j\}$ to construct an individual CCDF. For example, the consequence of the human intrusion scenario $\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E\, S_{drill})$ was combined with the probability of various numbers of intrusions into the repository using a discrete Poisson probability model, $\wp_{Poisson}\{\mathbf{p}^F,\mathbf{p}^E,S_{drill}\}$. Hence,

$$\wp\{\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E,\mathbf{p}^A) > R\} = \int_{p^E}\left[\sum_{j=0}^{nS} \mathcal{H}(\mathsf{R}(\mathbf{p}^F,\mathbf{p}^E,S_j)-R)\,\wp\{\mathbf{p}^F,\mathbf{p}^E,S_j\}\right] g(\mathbf{p}^E)\, d\mathbf{p}^E \tag{4}$$

The outer integration dealt with the epistemic parameter uncertainty. Characterizing the uncertainty in elements of $\mathbf{p}^E$ required developing a joint probability density function (PDF), $g(\mathbf{p}^E)$. The WIPP PA Analysts made the reasonable assumption that the individual parameters of $\mathbf{p}^E$ were independent and random such that the joint density function ($g(\mathbf{p}^E)$) was approximated by the product of PDFs of individual parameters $g(\varphi_1)\, g(\varphi_2) \ldots g(\varphi_n) \ldots g(\varphi_{nE})$. The procedure for developing $g(\varphi_n)$ for an epistemic parameter is the primary topic of this paper and discussed in Sections 3 and 4 below. Occasionally, $g(\varphi_n)$ was obtained by classical statistical techniques using field or laboratory data. However, in most cases, $g(\varphi_n)$ was based on subjective professional opinion obtained by informal elicitation of subject matter experts. Examples of both situations are described in a companion paper [17].

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[4] Obviously, the order of integration is immaterial and for practical reasons, the WIPP PA was set up as if the inner integration dealt with epistemic parameters (i.e., the WIPP PA first evaluated the function R for a particular scenario for all the uncertain epistemic parameters). However, the CCDF was assembled with the inner integration dealing with the aleatoric parameters as shown in Eq. (2) to develop a family of CCDFs in order to show the expected spread in results.

The Monte Carlo approximation of the outer integration used the specialized Latin Hypercube Sampling (LHS) technique [9; 54; 63; 64]. Each scenario configuration of the model, $R(\bullet)$, was run using a sample from the epistemic parameter class $\mathbf{p}^E$ to yield a sequence of *nLHS* results of the form $R_1(\mathbf{p}^F, \mathbf{p}^E, S_j), \ldots, R_{nLHS}(\mathbf{p}^F, \mathbf{p}^E, S_j)$. Then, the empirical CCDF was calculated as

$$\wp\{R(\mathbf{x},t;\mathbf{p}^F,\mathbf{p}^E,\mathbf{p}^A) > R\} = \frac{1}{nLHS}\sum_{k=0}^{nLHS}\sum_{j=0}^{nS} \mathcal{H}(R_k(\mathbf{p}^F,\mathbf{p}^E,S_j) - R)\ \wp\{\mathbf{p}^F,\mathbf{p}^E,S_j\} \qquad (5)$$

3. Parameter Development Team and Parameter Lead

To provide an estimate of the reasonably expected behavior of the WIPP, the assigned distribution of a parameter, φ_n, (either probability density functions [PDFs], $\mathcal{g}(\varphi_n)$, or cumulative distribution functions [CDFs], $\mathcal{G}(\varphi_n)$) should properly reflect the use in submodel $\mathcal{R}_\alpha(\bullet)$ or a probability model, $\wp\{\bullet\}$ developed by a PA Analyst. The distribution, $\mathcal{g}(\varphi_n)$, should also represent the best, current knowledge by a subject matter expert (SME) of the range and likelihood of the appropriate parameter value. Ideally, $\mathcal{g}(\varphi_n)$ would be assigned values based on applicable empirical evidence from laboratory and field experiments, but because of a frequent lack of empirical data, scientific literature and specialized knowledge of experts was usually required. To facilitate this parameter assignment, minimize bias, and assure reproducibility, a Parameter Task Leader was used in the 1991 PA and thereafter. Although not described in this paper, the parameter assignment for the 1996 PA was done under a formal QA plan with oversight by DOE, the EPA, and the State of New Mexico.

3.1 Parameter Task Leader Description

A rational assignment of a parameter distribution depends on both the form of the model in which it appears and the empirical data and other evidence available. Hence, both PA Analysts who need parameters for their model, and SMEs who provide relevant WIPP or literature information must jointly define parameters for a PA model. However, selecting the range and the distribution type, $\mathcal{g}(\varphi_n)$, for imprecisely known model parameters ($\mathbf{p}^E$) in a consistent manner that is sufficiently traceable for regulatory review, is a challenging task. Furthermore, in the WIPP context, the EPA Standard, 40 CFR 191 [27; 29], had called for "reasonable expectation" of the potential consequences of radioactive waste disposal at WIPP (Section 2.1); hence, parameter values (and models) were to be neither optimistically nor pessimistically biased. To achieve these goals, a key strategy was to appoint a Parameter Task Leader to oversee, mediate, and facilitate interaction between the PA Analyst and SME through the parameter development process (Fig. 4). The interaction of the SME with the PA Analyst, developed in 1990, is similar to the Kaplan's later recommendation to first elicit evidence from experts and then develop the distribution in conference with the experts rather than have the experts develop the distribution directly [24].

3.1.1 Responsibilities

The primary goal of the Parameter Task Leader was to provide guidance so that the myriad of parameter values and distributions (hereafter, simply "parameters") necessary in a PA were assigned consistently[5] and in an evenhanded fashion. In addition to this function, the Parameter Task Leader was responsible for developing a procedure to promote [14; 65]: (a) traceability (to ensure that a parameter used by the PA Department had a referenced source to provide a traceable link to underlying data); (b) retrievability (to ensure that a parameter can be easily retrieved for use in the computation model); (c) verification and parameter review (to ensuring that the parameters used were complete and consistent with PA model assumptions); and (d) documentation of parameters (to ensure that reviewers could readily understand the basis for choices on distribution type and the values).[6] Given the large number of tasks, the official title, Parameter Task Leader [14; 66], adequately described the position, but when considering the overall responsibility and authority of these tasks on the WIPP Project, peers commonly referred to the position as "Parameter Czar." However, rather than be dictatorial as the term "czar" might imply, ideally, the Parameter Task Leader was diplomatic with experience in the collection of experimental data, mathematical modeling building, and probability/statistics theory in order to provide meaningful guidance.[7]

3.1.2 Advantages

The 1979 Environmental Impact Statement (EIS) [68], 1989 Supplemental EIS (SEIS) [69], and 1989 PA [38] were conducted without a Parameter Task Leader (hereafter "Parameter Lead"), but even from this limited experience, several adverse situations became apparent. Without a Parameter Lead, the SME/PA Analyst interaction was haphazard: knowledge of developing parameter distributions was lacking in some interactions, experience gained from one parameter development effort was not readily passed on to others, and the interaction between the PA Analyst and SME was more easily dominated by a strong personality. With a Parameter Lead on the team in later PAs, the SME/PA interaction became more professional, timely, and documentation was more readily produced. Most importantly, the SME and PA Analyst more readily discussed whether the conditions under which data had been collected were applicable and representative of the conditions being modeled in the WIPP PA. Conceivably, a manager in the PA Department with statistical experience could perform the task of Parameter Lead, but the WIPP Project found that the use of a peer on the same management level as the PA Analyst and SME encouraged more fruitful interactions.

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[5] The WIPP Project worked on consistency to ensure that comparisons of parameter importance in sensitivity studies were valid much as an archer first works on consistently placing arrows in a tight cluster. Once consistency is obtained, accuracy is a much easier goal to reach. Since novel and perhaps better approaches are being explored, consistency and evenhandedness are not always necessary attributes in the scientific literature; however, they were quality attributes expected by the regulator for the WIPP engineering analysis.

[6] The NRC regulation for Yucca Mountain [32] specifically states (10 CFR 63.114): "Any performance assessment used to demonstrate compliance with § 63.113 must...(b) Account for uncertainties and variabilities and provide the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment."

[7] Parameter *Team* Leader, as adopted by the Yucca Mountain Project (YMP) [67] is a more appropriate description, in that it emphasizes the diplomatic nature of the position and yet correctly suggests numerous task responsibilities. It also recognizes that all the necessary qualities of the position may not reside in one individual.

3.1.3 Training by Parameter Lead to Avoiding Bias

Usually, the procedure was implemented through one-on-one interaction with the PA Analysts and SME and occasionally instructive memorandums [13; 15; 70; 71]. However, group meetings were useful. For instance, prior to the start of the 1991 PA, a day-long workshop was given to the PA Department and many of SMEs on the general methods of gathering information from experts. The workshop included a discussion of the five phases of the expert elicitation process (motivating, structuring, conditioning, encoding, and verifying) [21; 61; 65; 72; 73; 74] developed by the Stanford University/Stanford Research Institute during the 1960s and 1970s. Also, the attendees participated in a series of exercises to avoid overconfidence in estimating parameter distributions. Although not repeated in subsequent years, this initial training helped establish awareness within the WIPP Project of the importance of the parameter development process and the care that needed to be taken to avoid biasing parameter distributions and values.

When meeting with the Parameter Lead, an SME was occasionally unduly optimistic when asked to characterize the uncertainty in parameters and specified too narrow a parameter range. More often, however, the Parameter Lead found that an SME had the tendency to supply conservative values that would cause the results to appear less favorable than they should be (for at least those scenarios and situations that were foremost in the mind of the SME) as previously noted by Helton et al. [9]. Although the exercises in the 1991 workshop certainly reinforced this tendency to be cautious, it was clear that the tendency also prevailed among those SMEs who had come onto the WIPP Project late, had not participated in the workshop, and had not assimilated the culture of the project. Participants often had the mistaken notion that "conservative" models and parameters values were "more defensible" and thus results using these models and parameters were "more convincing."

However, conservatism was often not "more defensible" or "more convincing" at WIPP. First, parameters values that are conservative for all scenarios cannot be assigned in a complex system; hence, specifying a conservative value depends upon the scenario under consideration. An example of this situation was in the assignment of solute-transport parameters. Although specifying an unphysically high solubility and high colloidal transport fraction increased the removal of radioisotopes from the repository, specifying a high solubility and high colloidal transport fraction was clearly not conservative for evaluating the potential for nuclear criticality in and around the WIPP repository [75]. Hence, more than one value for solubility and colloidal transport fraction would have had to be specified with the accompanying potential to cause confusion unless realistic, consistent values were used. Second, and as pointed out in the literature numerous times [e.g., 37], maintaining a consistent level of "conservatism" for such a complex system is difficult. For example, in the 1989 PA, individuals had different notions of "conservatism." Furthermore, in a later prioritization study of proposed experiments [76; 1], excessive biasing to "game" the sensitivity analysis in an attempt to influence resource allocation was hard to control when conservatism was unwittingly allowed back into the analysis (see also Ref. [37]). Third, casual readers might not fully understand the concepts of a conceptual model and so an appeal to conservatism is futile. Furthermore, an appeal to conservatism can engender a suspicion that the model and parameters have not been developed using current scientific knowledge of the underlying phenomena.

Fourth, technically astute reviewers understand the concepts of a conceptual model but often want convincing evidence that the analyst can quantify how much uncertainty this component contributes to the overall uncertainty in the results. For example, the conceptual model (and corresponding parameters) for spalling of waste from the sides of a borehole during exploratory drilling was thought to be wildly conservative and thus "more defensible" by those analysts who constructed the model. However, the peer panel mandated by the EPA [30; 77; 78] to review the 24 major conceptual models[8] of the 1996 PA found this conceptual model to be the least defensible of the 24 because it could not be defended with scientifically based information and experimentally based parameter values [79]. Both the inability of the "conservative" model to match observed results in a simple experiment using wet sand without setting an empirical factor for capillary forces to zero and the inability to place the "conservatively" low parameter value used in the PA calculations for waste cementation, a parameter known to influence results, in context with measured values because of the lack of data, lead the panel to conclude the conceptual model was without "an adequate basis for determining that the Spallings model was either reasonable or conservative." Instead, the peer panel suggested that the WIPP Project develop a more realistic, mechanistic model of the spalling phenomenon and directly use measured data on waste characteristics [79] to quantify the suspected but unsupported conservatism of the model and parameter. Furthermore, because of this inadequacy of the spalling component of CUTTING_S [80], the EPA in their verification of the 1996 PA—"PA verification test" (PAVT) [81]—simply replaced the spalling component with a uniform distribution specifying waste volumes between 0.5 and 4.0 m^3 per spall event [78].

3.1.4 Management Categories of Parameters

When the parameter represented a physical process that had been studied during the characterization of the WIPP disposal system, the SME likely resided outside the PA Department. But a parameter might also represent some future condition such as the rate of exploratory drilling into the repository. For this situation, the "SME" resided within the PA Department and were handled by a PA Analyst since the EPA provided specific guidance for conducting the PA. To acknowledge the different sources of information, parameters tracked in the database were lumped into four broad categories that were separate and mostly distinct from the three classes of the parameter space previously introduced: (1) site or engineering specific parameters and, thus, dependent on information from WIPP investigators, (2) waste information parameters and, thus, dependent on information from reported inventory estimates [82], (3) precisely known, physical constant parameters, and (4) parameters representing future states of the WIPP and, thus, dependent on EPA guidance or the professional judgment of the PA Analysts. Code control

[8] The 24 major conceptual models (and associated parameters as discussed in a companion paper [17]) were as follows [77]: (1) frequency of drilling and location of plugs in exploratory borehole (Fig. 3); (2) conceptualization of brine pocket; (3) assumed chemical conditions in the repository; (4) dissolved concentrations of actinides in repository; (5) concentrations of colloids in repository; (6) two-dimensional, simplified disposal system geometry with one equivalent shaft and one intrusion borehole; (7) simplified disposal system geometry for multiple intrusions; (8) two-phase brine and gas flow conceptualization; (9) simplified Salado stratigraphy (Fig. 3); (10) use of impure halite properties for complex interaction of pure halite, clay, polyhalite, Fe-coatings, and anhydrite; (11) transmission of brines through and dilatation/fracturing of Salado anhydrite interbeds; (12) use of a fixed disturbed rock zone with high permeability and low porosity; (13) seal permeability and geometry of shafts and backfill; (14) conceptualization of gas generation; (15) representation of creep closure as a porosity surface; (16) advective/dispersive transport of actinides near repository without adsorption, colloidal filtering, and mineral precipitation; (17) actinide release via drill cuttings; (18) actinide release via spalling of waste into borehole; (19) actinide release via brine escaping directly to surface during drilling; (20) actinide release primarily via Culebra strata (Fig. 2); (21) conceptualization of Culebra transmissivity based on pumping tests; (22) dual (advective/diffusive) porosity model for dissolved actinide transport with adsorption in Culebra; (23) dual porosity model for colloidal actinide transport in Culebra; and (24) implementation of climatic change as multiplication factor on Culebra velocity field.

parameters (such as cell dimensions of a numerical grid and bounds on time steps) and model domain parameters were not tracked in the parameter database but represented a fifth category. The categorization helped from a management perspective in identifying and tracking whether the parameter was developed internal or external to the PA Department and, thus, the type of record files ("data packages") that were being developed [71]. As reported previously [9], out of the 1471 parameters, 409 parameters were based on site or engineering specific information developed by an SME, 89 were based on waste information,[9] 256 parameters were considered precisely known physical constants, and 717 parameters were based on professional judgment of PA Analysts. The difference methods for documenting the developed parameter distribution are neglected in the following description and so details of the management categories are not discussed further. The general process of assigning values and developing a parameter distribution, the emphasis of this paper, was followed regardless of the management category.

4. Parameter Development Process

Briefly, the parameter development process consisted of five steps discussed below (Fig. 5): (1) confer with PA Analysts on the parameters required for computational models used in the PA, (2) request data and other evidence from SMEs and discuss usage of parameter in PA computational models to help the SME provide appropriate and representative data, (3) construct a distribution, (4) place the parameter in the database and produce a parameter report or appendix documenting parameters, and (5) participate in planning discussions for future data collection and future analysis. The Parameter Lead first roughly followed these steps in the 1990 PA [11]. The steps were more formalized in a guidance report in the 1991 and 1992 PAs [14]; and in the 1996 PA, the steps became part of a formal quality assurance procedure [66].

4.1 Identify Computational Model Parameters

To begin the parameter-assignment process for newly developed computational models, the Parameter Lead and PA Analysts identified all constants and material-property parameters that were necessary to perform the simulations (Fig. 5). For the 1989 PA, the Parameter Lead simply collected information with minor consultation with SMEs. For the 1990 PA, the Parameter Lead set rough uncertainty ranges for parameters with more consultation. In the 1991 PA and thereafter, however, the SME become directly involved in the process. To avoid misunderstandings in interpretation by SMEs, a description of the models was included with the parameter reports after 1990 [13; 15].

[9] For the groundwater pathway (Fig. 3), all 89 parameters of total inventory for each radioisotope in contact-handled and remote-handled TRU waste placed in the repository were fixed [82]. Although some uncertainty existed in the total activity of each radioisotope, the 40 CFR 191 Standard scaled the releases by the total activity placed in the repository, and so this uncertainty was not of interest for comparison to the EPA limits. For the direct release pathway (Fig. 3), the variability from boring into a tiny subset of the 569 waste streams of contact-handled TRU waste was modeled and documented separately [82].

4.2 Request Pertinent Data from Project Investigators

At the request of the Parameter Lead through a memorandum, SMEs identified by the various Department Managers were asked to provide pertinent data for evaluating uncertain parameters[10] (Fig. 5). The SME extracted data specific to the natural or engineered barrier from WIPP experimental[11] databases and transmitted these data to the PA Department. The SME could supplement the WIPP-specific data with other data to fully characterize the uncertainty. For the 1990 PA and thereafter, the set of distributions and ranges developed for the previous PA, were distributed to the SMEs for their comment. For the 1990 [70], 1991 [13], and 1992 [15] PAs, SME recommendations were returned in the form of memoranda, which were published as appendices to a parameter report. For the 1996 PA, SME recommendations were recorded in parameter record packages and on a parameter entry form.

The most important information provided in the draft record package was a summary of existing measurements and evidence available; however, usually the SME went to the extra effort of providing an initial distribution for the parameter. Although the distribution might be modified when conferring with the Parameter Lead and PA Analyst, developing a distribution at this point was useful to further explain the intent of information and evidence provided by the SME. Furthermore, it might help to generate discussion. For example, in the 1991 PA, the SME (actually, a group of investigators represented by their supervisor) developed a distribution for the far-field pore pressure around the repository based on available measured data. The distribution included rather low measured pressures (1.1 MPa). Low measurements had been recorded in the depressurization zone near the repository, since the repository was open to the atmosphere. However, this minimum was not consistent with the intended use in the model, which, as pointed out by the PA Analysts, was to define a distribution for the far-field pore pressure prior to disturbance by the repository [13, A-133]. Hence, a subset of the data was used.

Although not directly related to this process, the quality of the data an SME might cite was of obvious importance. In 40 CFR 194 [45], the EPA required that the WIPP QA program meet the requirements of three QA standards of the American Society of Mechanical Engineers (ASME) [83; 84; 85]. It further implied that all data collected prior to the approval of the QA program by the EPA Administrator was considered existing data and had to be qualified. Information considered scientific fact (e.g., published information in reputable handbooks and textbooks) was classified as qualified data that needed no further review. The reasonableness in the use of other general scientific literature data cited was reviewed along with the overall review of the parameter records noted below in Section 4.

To qualify existing, WIPP-specific data, the project used two of four methods suggested by the EPA [45] and NRC [86]: (1) the project procedurally reviewed the QA program that existed during the collection of the data to determine if the existing program was essentially equivalent to the requirements in the three ASME standards, or (2)

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[10] As previously noted in Section 3.1.4, some model parameters were specific to the PA calculations and so individuals in the PA Department were considered the SME.

[11] Within the WIPP Project, the databases for WIPP-specific data under the control of an SME were called "primary" databases. Also, the database for parameter values under the control of the PA Database Administrator (Fig. 4) was called the "secondary" database since the parameter values were derived from the "primary" databases. Since the databases and their hierarchy are not of importance, herein we refer to them with slightly more meaningful terms to those outside the WIPP Project as "experimental" and "parameter" databases.

the project technically reviewed the adequacy of the experimental plans and procedures. The other two qualification methods suggested (qualification through confirmatory experiments on a small subset of the data and qualification through comparison with corroborating data that was collected under a equivalent QA program) were not used. The sequence followed was first to conduct a QA program review and then conduct a peer review, if necessary. To improve efficiency, the WIPP Project grouped similar data into 20 packages that were reviewed together. Fourteen data packages were found to have been collected under equivalent QA programs [71] and six data packages were decreed qualified after peer review. The QA program review committees was led by a specialist in Nuclear Quality Assurance (NQA) standards and consisted of one other QA specialist and one to three technical specialists. The peer review panels consisted of senior scientists. The review committees and panels also included an EPA observer. The members of the QA program review committees and peer review panels had no previous ties to the WIPP Project.

4.3 Assign Fixed Values

For the purposes of the WIPP PAs, three parameters types were designated fixed *a priori* (Fig. 5): (1) physical constants, conversion factors, and reference values, (2) code control, and (3) model domain parameters. The PA Analysts defined values for these fixed parameter types. A fourth parameter type, decision parameters concerning various experiment or design options (e.g., for internal management decisions on the value of funding future experiments) were also treated as fixed quantities after the 1990 PA but were developed in consultation with SMEs and thus followed the same path as uncertain parameters. All other parameter types were *initially* treated as uncertain. This statement does not mean to imply that all remaining parameters remained uncertain for clearly only 236 out of 1471 parameters had distributions assigned in the 1996 PA and of these 236 only 57 were ultimately treated as uncertain.

4.4 Elicit Parameter Values from Expert Judgment Panel

The degree of formalism used for the interpretation of primary (raw) data and any other related information to define parameter distributions can vary over a wide spectrum [14; 25; 65]. It ranges from interpretation by an individual with general knowledge of a given subject area, to individual interpretation by a recognized expert, to group interpretation by consultants, to formal elicitation of interpretations from a panel of recognized experts nominated by various stakeholders. The advantages of individual judgment are that (1) the work is much more rapid and much less expensive, (2) deep understanding of one subject can occur, and (3) there is personal ownership and thus likely a sense of craftsmanship in the judgment. The advantages of formally elicited judgments from a panel are that (1) it promotes clear and thorough documentation of how an interpretation was achieved, (2) it offers a structured procedure for gathering opinions, (3) it encourages diversity of opinion and, if conducted properly, minimizes bias and, thus, guards against understating or overstating uncertainties, and (4) it can bring together representatives of diverse disciplines to address interdisciplinary issues, which in turn, (5) initiates exchanges of ideas that would take many years to occur through the open literature. In three instances, formal expert judgment panels was formed for the 1991 and 1992 PAs: (1) to elicit how the rate of intrusion might change with time, (2) to

elicit the anticipated solubility of radioisotopes in the repository, and (3) to elicit adsorption coefficients [17]. In one instance, an expert judgment panel was used in the 1996 PA to elicit the particle diameter of waste when a hypothetical exploratory borehole enters the repository sometime in the future [87].

The Parameter Lead used the work of the panels and thus was a necessary supporting participant and presented information to the three panels. However, the size of the effort at WIPP precluded direct management of the expert elicitation process by the Parameter Lead even though the elicitation process was similar to that done informally with individual SMEs.

4.5 Construct Distributions for Uncertain Parameters

Except for those uncertain parameters that had been assigned distributions through an expert elicitation, the Parameter Lead selected/constructed or at least supervised the selection/construction of the distributions for uncertain parameters following several steps in consultation with the appropriate SME and PA Analyst [9] (Fig. 5). The assignment of values for parameters for which a distribution was not developed and were eventually fixed followed at least the first three steps. Even for eventually fixed parameters, a pessimistic or "conservative" value (or conversely, an optimistic value) was avoided since R(•) for the WIPP was too complicated to correctly determine a pessimistic value or the choice of a pessimistic value depended upon the scenario, S_j, being evaluated.

4.5.1 Step 1—Describe PA Model Parameters

As the first step, the PA Analyst described the pertinent PA model component and parameters (at first, orally in a team meeting and later by supplying documents such as the parameter report produced the previous year [13; 15; 70; 71]).

4.5.2 Step 2—Describe Data Available

In the second step, the SME described the data available concerning the particular parameter (possibly orally but usually through a memorandum in the preliminary PAs and in a parameter records package for the 1996 PA [13; 15; 70; 71].

4.5.3 Step 3—Evaluate Available Data

In the third step, the Parameter Lead examined the information available for specifying a parameter. If representative observational or literature data existed, the Parameter Lead went to Step 4; if no representative observational data were available, the Parameter Lead went to Step 5. The amount of time spent by the team on developing a distribution for a parameter in Step 4 or 5 was understandably dependent upon the importance of the parameter where the importance was either evaluated through past sensitivity studies or, for new parameters, the collective intuition of the team.

4.5.4 *Step 4—Develop Empirical Distribution*

If the number of values in the combined data set was three or more and representative (except possibly for the model scale), as defined by the SME, and at the appropriate model scale, as defined by the PA Analyst, the Parameter Lead used the combined data set directly to evaluate the parameter distribution. For example, data from permeability experiments of the Salado (Fig. 3) were used to develop an empirical, piecewise uniform PDF (see Section 5.3) in the 1991 and 1992 PAs. Historical data on drill bit diameters used in exploratory drilling in the Delaware basin (Fig. 1) were used to produce a discrete delta PDF (see Section 5.4) in the 1991 PA as described further in a companion paper [17]. Only for salt creep parameters [88] was data sufficiently abundant to enable a fit to the data and an evaluation of the goodness of fit[12] (i.e., either the chi-squared test or the Kolmogorov-Smirnov test). When the scale of the observational data was smaller than the modeling scale, the data could still be used but with additional interpretation. For example and as described further in a companion paper [17], a functional fit to available data combined with a boot-strap technique was used to explore uncertainty in the permeability of anhydrite in the far field of the Salado in the 1992 PA. In the 1996 PA, the Student-*t* distribution was used to represent the spatially averaged value for some parameters (described further in Section 4.8 and Appendix II). Otherwise, the Parameter Lead moved to Step 5.

4.5.5 *Step 5—Develop Subjective Distribution*

Often the SME had some observational information related to the model parameter, but the vexing question was whether or not the environment of measured or analogue data adequately represented the future environment of the WIPP disposal system. In this situation and others where observational data were lacking, the Parameter Lead asked the SME to provide subjective estimates of (a) if possible, the range of the parameter (i.e., the minimum and maximum values taken by the parameter with at least 99% confidence) and (b) if possible, one of the following (in decreasing order of preference): (1) percentile points for the distribution of the parameter (e.g., the 25th, 50th [median], and 75th percentiles), (2) the mean value and standard deviation of the distribution, or (3) only the mean value. Then, the Parameter Lead selected a distribution type depending upon the kind of subjective estimate that had been provided by using the maximum entropy formalism (MEF) discussed in Section 5: (a) a uniform PDF over the range of the parameter, $g_{uniform}(\varphi_n)$; (b) a piecewise uniform PDF based on the subjective percentiles, $g_{hist}(\varphi_n)$; (c) an exponential PDF (truncated) based on the subjective range and mean value, $g_{exp}(\varphi_n)$; (d) a normal PDF based on the subjective mean value and standard deviation, $g_{normal}(\varphi_n)$; or (e) a truncated normal PDF based on the subjective range, mean value, and standard deviation, $g_{trun\text{-}norm}(\varphi_n)$.

An alternative approach, noted in Fig. 5, which was used for several parameters in the 1989 and 1990 PAs, was to assign a distribution type based on what had frequently been used in the literature ("scientific precedence"). In

[12] Another parameter for which numerous data was available was matrix porosity of the Culebra ($\phi_{m\text{-}Culebra}$), which had been measured in 82 samples in 1989 and 103 samples by 1996. In 1989 and 1990, all samples were used to directly develop an empirical histogram PDF from which to calculate a mean and median value; however, because these core samples were only from between 20 (1991 and 1992) and 17 wells (1996), the 1991, 1992 and 1996 PAs, more correctly averaged porosity values from each well and then used the 20 or 17 averages to develop a empirical histogram distribution.

the 1989 and 1990 PAs, the permeability (k_x) of the abandoned borehole, and the permeabilities of halite and anhydrite layers of the Salado (Fig. 3) were assigned truncated lognormal PDFs; the waste porosity[13] (ϕ_m) was assigned a truncated normal PDF. Although others continue to suggest this approach (e.g., Ref. [89]), the reasoning for other distribution types used in the literature (except for normal or lognormal distributions) was often not strong. This fact coupled with the flexibility of the piecewise uniform PDF caused this alternative approach to be abandoned in later PAs.

If necessary, steps 1-5 were repeated until a meaningful distribution was produced. Although the Parameter Lead was responsible for guiding the development of the distribution, ideally, the process only ended when all three participants, the Parameter Lead, PA Analyst, and SME, could agree. However, disputes did occasionally occur. Prior to the 1996 PA, the participants could agree to disagree, the Parameter Lead would decree the parameter distribution based on his judgment or occasionally acquiesce to the SME or PA Analyst judgment, and then the participants would wait until the next iteration to see if the SME had better information that might resolve the dispute. For the 1996 PA, much more effort was spent on reaching an agreement: signatures on a parameter entry form documented this agreement[14] and represented an important project milestone. In one instance, an internal mediator was called in to help structure concurrence on how to use both laboratory and field data for evaluating the anhydrite permeability in the Salado [71, Appendix J] as described further in companion paper [17]; however, resolution through management decree was avoided.

4.6 Document Parameters

For the 1989 PA, the parameter documentation consisted of a table in the main report [38, Table 3-9] for the uncertain parameters propagated through the analysis and appendix for the remaining uncertain but fixed values in the analysis [90]. For the 1990, 1991, and 1992 PAs, the Parameter Lead prepared parameter reports [13; 15; 70], that described the general process and reasoning used to select parameter values and distributions (Fig. 4). An appendix contained the memorandums from the SME on the background information and initial recommendations.

The parameter database for the 1989 PA consisted of an ASCII text file. Thereafter, commercial database software (INGRES®) was used to allow easy sharing of the parameter values among multiple users and multiple applications, but the parameter values were still organized as simple tables. A Data Administrator was responsible for updating the parameter database with the endorsed information. After the database was updated, the Parameter Lead (Fig. 4) authorized the creation of an ASCII output file (a "view" of the database from INGRES®) for use in PA simulations. The codes to sample distributions (LHS [64]) and set fixed parameter values (MATSET [91; 92]) accessed this ASCII output file through a series of software routines.

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[13] All parameters were defined by a parameter character name that was associated with a material character name in the WIPP Parameter Database (e.g., PRMX_LOG and BOREHOLE—Ref. [71], App. A; [4], App. PAR). In addition, when describing the sampled parameters, Helton et al. [9, Table 1] defined a new parameter character name that linked the parameter name and material name to be more succinct (e.g., BHPRM). Finally, the articles describing the 1996 PA used a set of symbols that differs somewhat from the symbols used herein. An attempt was made to place all three sets of nomenclature in Appendix I when listing the symbols used in this paper to help clarify the meaning of the symbol.

[14] In addition, the parameter entry form eliminated the need for the Data Base Administrator (Fig. 4) to view the record package developed by the SME since essential parameter information had been recorded on the parameter entry form.

For the 1996 PA, the Parameter Lead submitted a completed Parameter Entry Form to the Data Administrator following the successful development of a distribution. The Parameter Entry Form was the primary source document listed in the database to which other data sources could by tracked. In addition, a summary description of the uncertain parameters was documented in an appendix to the CCA (Ref. [4], Appendix PAR). Furthermore, in place of a memorandum on background information for the parameter, the SME was responsible for producing a record file on (a) background information pertinent to the parameter, (b) the rationale for the choice of specific data to use in the development of the parameter, and (c) references to other pertinent record files (e.g., records containing the collected data). Generally, the record file underwent a standard technical review and the supporting records that contained the specific data collected underwent the QA program and possibly peer review mentioned in Section 4.2. The specific type of record file created depended upon the management category of the parameter mentioned in Section 3.1.4. For example, when the SME was actually the PA Analyst within the PA Department, the record file on the parameter could be included as part of the record file describing the submodel, $\mathfrak{R}_{\alpha}(\bullet)$ and corresponding analysis.

4.7 Plan PA Simulation and Assess Parameter Importance

The Parameter Lead was involved in discussions within the PA Department on selecting those parameters whose uncertainty should be propagated through the analysis (i.e., parameters "to sample") (Fig. 6). In general, if the coefficient of variation ($\sigma_{\varphi}/\mu_{\varphi}$) or range [$a_{\varphi}$, b_{φ}] of the distribution was small (i.e., $\sigma_{\varphi}/\mu_{\varphi} < \sim 0.1$ or $b_{\varphi}/a_{\varphi} < 1.3$) on the linear scale, the WIPP project treated the parameter as constant. However, these criteria were not sufficient to preclude propagating the parameter uncertainty since parameter importance is actually dependent on the relative sensitivity of the various models used in the WIPP PAs (i.e., b_{φ}/a_{φ} or $\sigma_{\varphi}/\mu_{\varphi}$ could not be used as a surrogate for estimating the importance of parameter uncertainty in explaining uncertainty in the performance measure results). For example, the square of the diameter of the inadvertent human intrusion borehole is linearly proportional to the waste cuttings removed in an intrusion at WIPP. Furthermore, the release of radioisotopes through this cuttings pathway has dominated the overall releases in all PAs [1, Figure 16]; hence, the diameter of the intrusion borehole was always an important parameter. In the 1990 PA, the CUTTING submodel, $\mathfrak{R}_{CUTTING}$ [70; 80; 88; 92] (Fig. 3), used the removal area as a parameter and a distribution was developed based on the historically used diameters for exploratory drill holes in the Delaware Basin (Fig. 1). For this piecewise uniform PDF of drill-hole area, b_{φ}/a_{φ} = 13.5. However, in the 1991 and 1992 PAs, $\mathfrak{R}_{CUTTING}$ was modified slightly and the drill-hole diameter was used directly. Although the range of the drill-hole area was large, the range of the distribution for the diameter was narrow (a uniform PDF between 0.267 and 0.444 m, b_{φ}/a_{φ} = 1.7 and $\sigma_{\varphi}/\mu_{\varphi}$ = 0.14). Therefore, the criteria were not used solely to select parameters to analyze the contribution of their uncertainty to the uncertainty in the results. Instead, the criteria were used as a rough rule-of-thumb that alerted the Parameter Lead that more thought might be in order before selecting a particular parameter for study. When a parameter was important, yet $\sigma_{\varphi}/\mu_{\varphi}$ or b_{φ}/a_{φ}, were small, the criteria also served to alert PA Analysts that more study was warranted to see if a possible error had occurred in the calculation or, less likely, the submodel exhibited strong nonlinearities.

After the analysis, the PA Department used the PA results and specification of parameter uncertainty for future planning and project decisions. The distributions for parameters found important in at least one of the WIPP PA iterations are discussed in a companion paper [17].

4.8 Repeat Process for Each Iteration

The distribution-development process started over for each iteration of the PA (Fig. 5). The understanding about the importance of various FEPs in the disposal system increased because of the PA iterations, and consequently, the SME and PA Analyst could more carefully consider the available information and use of the parameter in the PA with deeper understanding. Although conceivably parameter distributions could have been assigned through Bayesian updating in later iterations, this was not done for several reasons. First, the meaning of many parameters changed between iterations. For instance, the role of the solubility parameter changed as major model updates were made between the 1989 PA and 1991 PA, as described in a companion paper [17]. Second, experimental techniques greatly improved and so the ranges of distributions changed. For example, the capability to measure the low permeability of the halite in the Salado (k_x) improved dramatically over the course of the WIPP Project [1; 5; 17]; hence, the minimum permeability for the distribution decreased by 4.5 orders of magnitude. Finally, substantially new data often did not become available between early iterations. For example, substantially new data did not become available during the first four PAs for solubility and adsorption coefficients (Kd) of radioisotopes [17].

A by-product of repeating the distribution-development process was to improve the interaction between the three-team members—SME, PA Analyst, and Parameter Lead. Examples include the improved description of mathematical models in project documents and the already mentioned workshop training for the 1991 PA.

5. Selection of Distribution Types

There were two goals in developing a distribution from available data and information: (1) provide an easily understood rationale for the distribution (through consistent use of objective techniques that are easily understood by others), and (2) minimize SME bias (by employing techniques that make direct use of what is known and only what is known). The primary approach for meeting these two goals was the series of steps described above in Section 4. Yet, as described below, guidance on the use of a logarithmic transform and the maximum entropy formalism (MEF) helped to consistently select a range and distribution type.

5.1 Log Transform

Many continuous distributions converge to a similar shape as the coefficient of variation of the distribution ($\sigma_\varphi/\mu_\varphi$) becomes small. Indeed, distributions are already remarkably similar [21, Figure 5.4] for $\sigma_\varphi/\mu_\varphi = 0.2$ and, thus, the Parameter Lead did not expend much effort on selecting distribution types for $\sigma_\varphi/\mu_\varphi \leq 0.2$ (see Section 6.3 on sensitivity of results to distribution types). Furthermore, and as already noted in Section 4.7, the WIPP project usually fixed a parameter value whenever $\sigma_\varphi/\mu_\varphi < \sim 0.1$ where σ_φ and μ_φ were evaluated on the linear scale. Yet, understandably a log transform of the parameter before assigning a named PDF (e.g., uniform or normal) can

strongly influence results. Hence, to establish a degree of consistency, a distribution in linear space was usually used when the parameter range spanned less than an order of magnitude[15] ($b_\varphi/a_\varphi \leq 10$ or if $a_\varphi = 0$, $b_\varphi \leq 10$), and a logarithmic transformation was usually used when the parameter range spanned two or more orders of magnitude (i.e., $b_\varphi/a_\varphi \geq 100$ or if $a_\varphi = 0$, $b_\varphi \geq 100$).[16] Between the one and two order of magnitude range either a linear or logarithmic transformation was used at the discretion of the Parameter Lead. Although not published during the time of the WIPP PAs, others provided somewhat similar guidance. The NCRP [61] stated that when the range of uncertainty exceeded a factor of 10 or $\sigma_\varphi/\mu_\varphi > 0.3$, it is often prudent to use a logarithmic transform.[17] Herein, the term "log" in front of a named PDF or piecewise linear PDF, indicates that the distribution was assigned on the log-transform of the parameter values.

5.2 Maximum Entropy Formalism

Although the connection between probability and uncertainty is implicit, Shannon in 1948 (e.g., Refs. [20]; [19]) quantitatively defined the connection using a "measure of information" or "informational entropy," $U(\varphi_n)$ equal to $-\int g(\varphi_n)\, ln\, g(\varphi_n)\, d\varphi_n$ for continuous distributions or $-\sum \varphi_n\, ln\, \varphi_n$ for discrete distributions. In 1957, Jaynes described a maximum entropy formalism that stated that of all the distributions that can be chosen based on the information at hand, the one distribution that maximizes $U(\varphi_n)$ is the least prejudiced or least biased selection (e.g., Refs. [19]; [20]). Hence, using this maximum entropy formalism (MEF) or principal, a unique PDF can be determined that maximizes $U(\varphi_n)$ while satisfying prescribed constraints. These constraints can be such things as a known mean and known standard deviation. The literature on selecting a distribution, given various kinds of constraints, was vast by 1990 [18]; thus, almost all the results needed by the WIPP team were reported in the literature; in only one case (constraints in the form of given quantiles) was it necessary to develop the MEF distribution (Appendix III).

Further, only a small set of MEF distributions was needed for the WIPP parameters. These PDFs included delta functions for discrete parameters, and the uniform, piecewise uniform, truncated normal, Poisson, and exponential distributions for continuous parameters. In addition, two other non-MEF distributions were used at times: beta in the 1989 PA and triangular in the 1996 PA (Table 1). The two most common distributions used for describing parameter uncertainty were the uniform and piecewise uniform PDF (Fig. 7).

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[15] For WIPP, all parameters were zero or greater on the linear scale; hence, the ratio b_φ/a_φ was always positive.

[16] These were general guidelines. For two subjective parameters, shear strength of waste when borehole intrudes into the repository ($\tau_{fail\text{-}waste}$) [80; 17], and multiplier for transmissivity field after mining for Potash below the Culebra ($f_{mine\text{-}trans}$) [53; 17], a linear scale for the uniform distribution was used but $b_\tau/a_\tau = 200$ and $b_f/a_f = 1000$, respectively, in the 1996 PA. Also for the adsorption coefficient for U^{VI} (Kd_{UVI}) [9; 17], $b_{KdU}/a_{KdU} = 1000$; however, a linear scale for the uniform distribution was used since all other adsorption coefficients had $b_{Kd}/a_{Kd} < 100$.

[17] For uniform and truncated normal distributions, a range of two orders of magnitude corresponds to a coefficient of variation near 0.5 (i.e., if $b_\varphi/a_\varphi = 100$, then for uniform distribution, $\sigma_\varphi/\mu_\varphi = [(b_\varphi - a_\varphi)/2\sqrt{3}]/[(b_\varphi + a_\varphi)/2] = (1/\sqrt{3})(99a_\varphi/101a_\varphi) \cong 0.56$, and for normal distribution truncated at $\mu_\varphi \pm 2.33\sigma_\varphi$ (99% of distribution) then $\sigma_\varphi/\mu_\varphi = [(b_\varphi - a_\varphi)/4.66]/[(b_\varphi + a_\varphi)/2] = (1/2.33)(99a_\varphi/101a_\varphi) \cong 0.42$.

5.3 Subjective Uniform Distribution

The uniform PDF [93] was typically selected when all that was known or estimated about a parameter (either in linear and log space) was its range (a_φ, b_φ). The uniform PDF is an MEF under these circumstances [19; 20]. The maximum coefficient of variation (σ/μ) for a uniform PDF in linear space is 0.58. This distribution was useful as a default for sensitivity studies and was the distribution usually chosen when a parameter was first introduced into the PA process. For example, over 58% of parameters tracked in the parameter database in the 1989 PA were assigned a uniform PDF. Thereafter, the number of uniform distributions assigned remained at about 20% or higher throughout the PA iterations (Fig. 7). Conceivably, data could be "fit" to a uniform distribution by the method of moments (i.e., $a_\varphi = \mu_\varphi - \sqrt{3}\ \sigma_\varphi$, $b_\varphi = \mu_\varphi + \sqrt{3}\ \sigma_\varphi$); however, if representative empirical data were available, a piecewise uniform "histogram" PDF was used, as described in the next section. More importantly, parameter values were not typically measured directly in an experiment and so the SME had to interpret the data to fit the context of the mathematical model being used in the WIPP PA as emphasized several times throughout this paper.

5.4 Subjective and Empirical Histogram and Discrete Distributions

The piecewise uniform PDF (sometimes referred to a piecewise linear CDF[18] and succinctly termed a "histogram" PDF hereafter) is the maximum entropy distribution (see Appendix III) for a parameter that is continuously distributed but defined with a set of percentile points $(\varphi_1, \wp_1)$ $(\varphi_2, \wp_2)$,..., $(\varphi_n, \wp_n)$, independent of whether the percentiles ($\wp_1$, $\wp_2$,..., $\wp_n$) are empirically or subjectively derived.[19] In 1990 through 1992, over 60% of the distributions were histogram PDFs (Fig. 7b). These histogram PDF were obtained by (1) plotting the subjectively determined percentile points from professional judgment or formal expert elicitation; (2) plotting empirical percentiles of data, or (3) in two cases, simulating the distribution by kriging and bootstrap techniques [17].

One potential advantage of the histogram PDF is that if the number of quantiles specified is sufficient, a log transform of the parameter does not have a strong influence on a histogram PDF. For example, in 1991, the element solubility (S_e) and the adsorption coefficient (Kd_e) were specified on the linear scale with between 7 and 10 quantile points. In 1992, the log transform of the *same* quantile points was used. This change altered the mean of the distribution only slightly, and there was no discernable impact on the performance measure result [17].

For the cases where a histogram PDF represented empirical data, the Weibull plotting position was used (i.e., $\wp\{M < m\}$ = cumulative frequency = $m/(n_{sample}+1)$ where m is the rank of the value of interest and n_{sample} is the total number of sample points) [95, Table 7.4]. We do not know whether an empirical histogram PDF based on samples of a continuous random variable is an unbiased estimate of the underlying distribution.

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[18] Within the WIPP Project, it was most often called "piecewise linear CDF" [11] and identified in the WIPP database as "cumulative" since it was the only distribution identified in CDF space [94; 71]. To be consistent with the nomenclature of other distributions where the PDF is named rather than the CDF, the WIPP literature described the distribution as "piecewise uniform PDF," [e.g., 9]. We have coined the equally descriptive but short name "histogram" PDF here. Also in 1991, the distinction between a subjective and empirical histogram PDF was maintained; the latter empirical histogram PDF was identified in the database as "data." [13].

[19] Conceptually, the piecewise uniform PDF is a discretization of a PDF. This discretization provides the parameter development team the same flexibility as spatial discretization in a finite-element or finite-difference numerical model provides a PA Analyst.

For the preliminary PAs, an important aspect was the sensitivity analysis that guided future data collection efforts (Fig. 6). Further, since the range of the distribution was important to determining sensitivity, the PA Department was concerned about prematurely decreeing a parameter unimportant and thereby curtailing further work in 1990 and 1991; hence, in addition to the empirical data, the PA Department either asked the SME to provide either an upper and lower bound to the measured data or produce a default upper and lower bound based on the sample σ_φ (i.e., the issue of experimental and model scale was neglected). The default bounds were $\mu_\varphi \pm 2.33\sigma_\varphi$, which represented 98% of a normal distribution, 92% of a unimodal, symmetric distribution based on Gauss' inequality, and > 82% for any other distribution, based on Chebyshev's inequality [20]. In addition, the lower limit of the distribution was not allowed to be less than zero for an intrinsically positive parameter and both the lower and upper bound were not allowed to exceed physical limits. For example in the 1991 PA, the default upper bound for the far field pore pressure in the anhydrite Marker Bed 139 directly below the repository (Fig. 3) exceeded the lithostatic pressure of 15 MPa and was thus reduced to this physical limit [13, p. A-133; 17]. For the 1996 PA, the emphasis on defining the distribution shifted to the issue of defining the best possible representation given the data at hand; hence, the question of the difference between experimental and model scale became important and a Student-*t* distribution was used as explained below in Section 5.8.

A discrete distribution defined by a set of percentile points $(\varphi_1, \wp_1)$, $(\varphi_2, \wp_2)$,..., $(\varphi_n, \wp_n)$, independent of whether the percentiles $(\wp_1, \wp_2, \ldots, \wp_n)$ are empirically or subjectively derived, was succinctly called a delta PDF (piecewise uniform or "stair-step" CDF) herein. A delta PDF for a discrete parameter could be a maximum entropy distribution for a discrete parameter, depending on various circumstances. In the 1990 PA, the discrete delta PDF described the possible future exploratory drill-hole diameters based on the historical use of exploratory wells in the Delaware basin [17; 70] (Fig. 1). In 1996, the discrete delta PDF described the probability of two alternative conceptual models for relative permeability (Brooks-Corey or van Genuchten-Parker) for several materials in the two-phase flow simulation [9; 51] (Fig. 7). Although a sample mean can be calculated for a discrete delta PDF, the mean is often not equal to one of the discrete values and must be approximated by the nearest discrete value. Similarly, the median $({}^{50\%}\varphi_n)$ was approximated by the nearest discrete value at the 50% point on the stair-step CDF.[20] An empirical delta PDF based on samples of a continuous random variable is an unbiased estimate of the underlying distribution [96].

5.5 Subjective and Empirical Normal and Beta Distributions

The normal PDF [97] is a maximum entropy distribution [19; 20] given the mean (μ_φ) and variance of φ_n (σ^2_φ). Based on the central limit theorem [98], the use of the normal distribution is appropriate whenever it is known that the parameter is the sum of independent, identically-distributed random variables (e.g., addition of many small

[20] In the 1989, 1990, 1991, and 1992 PAs, usually the mean of the distribution was used when the parameter was fixed. In addition, the WIPP Project conducted simulations using only mean or median values for those parameters varied in the analysis. These two deterministic simulations were made in order to compare the results with the mean and median determined from the Monte Carlo simulation. This comparison allowed the PA Analysts to qualitatively evaluate the overall degree of nonlinearity in the modeling system [21]. Because the radioisotope releases via cuttings and cavings gradually dominated the total releases and were a linear function of the amount of waste brought to the surface, the nonlinearity of the modeling system gradually decreased in each PA iteration.

effects) and when there are a sufficient number of measurements of the parameter [$n_{sample} > 10$] to make, reasonably precise, unbiased estimates of μ_φ and σ^2_φ.

The truncated normal is the MEF distribution when the range is given in addition to μ_φ and σ^2_φ. In the WIPP PAs, ranges of uncertain parameters were always bounded to avoid sampling unphysical values in sensitivity and uncertainty analyses. As a starting point, the bounds for normal or log normal distributions were assumed to occur at the 0.01 and 0.99 quantiles, which corresponds to $\mu_\varphi \pm 2.33\sigma_\varphi$. This interval corresponds to 98% of the distribution, slightly more than the common 95% confidence interval.[21] Certainly, estimating a 99% confidence interval (quantiles at 0.005 and 0.995) would also have been fairly reasonable, but the usual consensus of the parameter development team was that estimating a confidence interval any larger than 99% was beyond the capability of the team to meaningfully estimate without directly applicable experience. Of course, physical constraints were observed such that intrinsically positive variables were bounded below by zero. Yet, even without obvious physical constraints, the parameter development team, had to decide, based on the available data (as described by the SME) and the use of the parameter in a model (as described by the PA Analyst), the reasonableness of these default bounds.

The beta PDF [20; 93] is a versatile density function that can assume numerous shapes in a specified range. The beta PDF is defined based on a specification of a range (a_φ, b_φ), μ_φ, and σ^2_φ. It provides a slightly different shape than the truncated normal MEF distribution, thus, it was only used initially in the 1989 PA and for four unsampled distributions in 1990 (Fig. 7).

For those parameters that were varied in the 1989 PA [38], any available data was usually fit to either normal or beta distributions as follows (i.e., the 1989 PA used a more ad hoc approach by selecting distributions frequently used in the literature [Section 4.4.5—Fig. 5] and did not consider the representativeness of the data): (1) for porosity, a normal distribution was tried; if the normal PDF had an inadequate fit, a lognormal PDF or beta PDF was used; (2) for hydraulic conductivity, a lognormal PDF was tried; if the fit was inadequate, then a beta PDF was used; (3) for radioisotope retardation, a beta distribution was required to fit the available data. In the end, the majority of 27 sampled distributions in the 1989 PA were normal (Fig. 7a). Thereafter, the number was < 10%. This 10% included the intrusion borehole permeability ($k_{x,bore}$) and measurement errors. The EPA Standard, 40 CFR 191 [27; 29], specified that the intrusion borehole permeability was to be that of sand and so a textbook mean value [100] and truncated lognormal PDF was assumed in all PAs. In addition, errors that might occur when measuring heads ($H_{freshH2O,well}$) and transmissivity ($\mathfrak{T}_{K,well}$) in field well tests of the Culebra [17; 53] were assumed to be normally distributed to develop spatial fields of heads and transmissivity values through kriging in the 1992 and 1996 PAs [101]. In general, to encode the SME's beliefs about the value of a parameter by manipulating the mean (μ_φ) and variance (σ_φ) to define a normal PDF for a parameter was too inhibiting and so was eventually discouraged. Most SMEs found that they could not supply reasoned estimates of μ_φ if the distribution was skewed or reasoned

[21] The Intergovernmental Panel on Climate Change (IPCC) of the United Nations suggested that estimated bounds represented 95% of the distribution ($\mu_\varphi \pm 1.96\sigma_\varphi$) when describing the uncertainty in national inventories of greenhouse gases [99].

estimates of σ_φ in the absence of similar data.[22] Rather, the use of a subjective histogram distribution discussed above was favored in later PAs.

5.6 Subjective Exponential and Poisson Distributions

In 1990, the human intrusion event through exploratory drilling (representing aleatoric uncertainty in the WIPP PAs) was (a) modeled as a separate scenario, and (b) simulated as part of an overall analysis. In the case of the simulated intrusion, the connectivity was based both on time and the location of the multiple intrusions in the repository. After 1990, Sandia did not include the intrusion as part of a full simulation, but only as a separate scenario. In the case of the separate scenario, the probability of various intrusion situations (i.e., one, two, or more intrusions and the borehole connectivity (i.e., communication of flow through the repository between the abandoned boreholes) were calculated independent of the consequence analysis and based on time between intrusions (time bins) [57; 62].

In both cases, the mean rate of intrusion and the mean waiting time between intrusions were specified. Initially, the EPA Standard, 40 CFR 191 [27; 29], specified[23] the mean rate of human intrusion (λ_{drill}) into a repository in sedimentary rock as 30 boreholes/km^2-10^4 yr. Given only a mean λ_{drill}, the exponential PDF [97], which preserves maximum entropy, was used to define the time of the first intrusion in 1990 and thereafter (Fig. 7). Similarly, in 1990, the WIPP Project assumed that the mean waiting time between intrusions was $1/\lambda_{drill}$; hence, the maximum entropy Poisson PDF [102] was used to define the number of intrusions that could occur in any specified period. After 1990, the WIPP Project continued to assume that human intrusion was a Poisson process [57] but this fundamental assumption was built into the software assembling the results of and probabilities from the various scenarios into a CCDF and so Poisson and Exponential PDFs were no longer explicitly sampled (Fig. 7).

5.7 Subjective Triangular Distribution

The measure of central tendency that most SMEs could supply was either the median (${}^{50\%}\varphi_n$) or subjective mode (${}^{max}\wp_\varphi$). In the 1996 PA, the SME responsible for defining parameters for the engineering material for backfilling the shaft and underground drifts felt most comfortable specifying a mode rather than a median value (in addition to the range) for the permeability tensor for 9 of the 10 materials [103]. For the crushed salt material of the shaft, the permeability was also assumed to change with time. In all, 43 permeability triangular PDFs were defined for the shaft backfill [71] (Fig. 7). However, all original materials were assumed to be homogeneous and isotropic and so while permeability was defined in three spatial directions, a single PDF was sampled and the value applied to each direction.[24] Also, triangular PDFs were used to define the pressure, compressibility, and permeability of the Castile

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[22] When data are available for a parameter and the parameter has been measured frequently, a characteristic coefficient of variation (μ/σ) is often observed [20, Table 1.8.1], but this situation was not the case for parameters used in models at WIPP.

[23] Later, the implementing regulation for WIPP, 40 CFR 194 [43], required the DOE to evaluate the drilling rate that had occurred over the last 100 yr for both shallow and deep exploratory wells in the Delaware Basin as described in companion paper [17].

[24] The modeled permeability of the shaft backfill was the combination of the specified permeability of the backfill in the four shafts (air, exhaust, salt, and waste) and the permeability of the disturbed rock zone around the shaft, weighted by the corresponding distances $r_{air\text{-}shaft}$, $r_{exhaust\text{-}shaft}$, $r_{salt\text{-}shaft}$, $r_{waste\text{-}shaft}$, $r_{DRZ\text{-}shaft}$. Hence, the effective permeability of the shaft was homogeneous but anisotropic.

brine reservoir (5 addition triangular distributions). Thus, although a total of 48 triangular PDFs were defined, only 12 were unique (3 triangular PDFs in the Castile brine reservoir (Fig. 3) where 2 were almost symmetrical and one, the pressure, had a mean of 13.6 MPa and mode of 12.7 MPa, 5 almost symmetrical triangular PDFs for permeability of shaft disturbed rock zone, earthen fill, clay, asphalt and concrete of the shaft, and 4 almost symmetrical triangular PDFs for the permeability of the crushed salt backfill at 4 different times).

In the absence of additional information about the probability value of the triangular PDF at the mode (information usually not known), the use of a mode as a constraint in the MEF only gives back the uniform PDF over the range (a_φ, b_φ), the same distribution that arises if the range alone is specified. More importantly, the triangular PDF is not as flexible as the histogram PDF in accommodating additional qualitative information and degrees of belief about length and shape of the tails of the distribution that is revealed during discussion and review by the parameter development team (Fig. 4); hence, the Parameter Lead discouraged the use of the triangular PDF. When an SME wished to taper the distribution at the tails, an SME could easily use a few intermediate quantiles (e.g., 0.75 and 0.90 quantiles) to mimic the tapering behavior of a triangular PDF.[25]

In the situation at WIPP, the triangular PDFs for permeability were defined in log space, and in all cases, the coefficient of variation ($\sigma_{log(k)}/\mu_{log(k)}$) for the logarithmic transform of permeability was less than 0.1. Consequently, the precise shape of the permeability distribution was not important, as discussed previously in Section 4.1, and the parameter development team was most interested in defining the range of the distribution.[26] Furthermore, release through the sealed shafts had never occurred before; thus, the team allocated their time to defining distribution types of other parameters that had been found important in previous PAs.

5.8 Student-t Distribution

The WIPP Project used the Student-*t* distribution [93] to quantify uncertainty in those parameters that specified spatial averages of heterogeneous geologic rock properties in the model (such as permeability, porosity, and fracture density) and some human-produced materials (such as TRU waste) (Fig. 7). The *t* distribution is appropriate when one must specify an effective value for an intensive material property in a numerical model (finite-element or finite-difference) and the sizes of the elements (or cells or zones) are much larger than the size of experimental measurements. The difficulty in characterizing heterogeneous geologic media properly to reflect the scale of the model and spatial variability, in addition to any other epistemic uncertainty, was a unique aspect of PA analysis for the WIPP that set it apart from other large-scale modeling such as a PRA for an engineered nuclear reactor. A

[25] As noted in 1962 [104] and recently discussed by Scherer et al. [105], the symmetrical triangular PDF provides a good approximation to the normal PDF with known μ and σ. Hence, when one defines the uncertainty of a parameter with a symmetrical triangular PDF, conceptually, one is approximating a normal (or truncated normal) distribution. For the WIPP PA, there was no computational advantage to using a triangular PDF to approximate a parameter with a known normal or lognormal PDF. In the cases where the SME provided almost symmetrical triangular PDFs, the Parameter Lead could have readily converted them to normal PDFs. Similarly, the one mildly unsymmetrical triangular PDF of Castile brine pressure could have been converted to an equivalent lognormal PDF.

[26] Although $\sigma_{log(k)} / \mu_{log(k)} < 0.1$ in logarithmic space where the distributions were defined, in linear space where the parameters were actually used, $\sigma_k / \mu_k > 0.1$; hence, the permeability of the shaft disturbed rock zone and shaft backfill (crushed salt, clay, asphalt, and concrete) were valid candidates for evaluating uncertainty and were sampled in the 1996 PA.

mathematical justification for using the t distribution is described in Appendix II; this justification is summarized briefly here.

Inferences about the appropriate parameter values to use while properly considering model-scaling issues (i.e., the choice of conceptual model, material zones, and numerical grid) made use of the following two observations. First, the variance of any material-property parameter, φ_n, in the large-scale PA model was less than or equal to the apparent variance of the material property at the local measured scale (i.e., $\sigma_{local}(\varphi_n) > \sigma_{element}(\varphi_n)$). As argued in Appendix II, the variance of φ_n, $\sigma^2_{cell}(\varphi_n)$ is

$$\sigma^2_{cell}(\varphi_n) \cong (V_{local}/V_{cell})\sigma^2_{local}(\varphi_n) \quad (1)$$

where V_{cell} is the volume of the numerical cell or element over which the material property is to be averaged and V_{local} is the volume over which the material-property parameter is correlated in the field. Although the volume of correlation (V_{local}) was not precisely known, it was often known that the correlation volume $V_{local} << V_{cell}$ such that the variance of the volumetric averaged parameter ($\sigma^2_{cell}(\varphi_n)$) was much smaller than the variance of the parameter measured on a local scale ($\sigma^2_{local}(\varphi_n)$). In other words, the variability of φ_n at the local scale that was estimated by the experimental samples had a much larger variability than would be anticipated at the scale of one numerical cell of the model.

Second, if the expected value of a property in the element was the mean of the local observations (i.e., $\mu_{local}(\varphi_n)$), then one must estimate the uncertainty inherent in estimating the mean $\mu_{local}(\varphi_n)$ that arises from (1) a limited number of measurements of the material property, and (2) the correlation that may occur between $\mu_{local}(\varphi_n)$ and other uncertain parameters φ_m of the PA model. At WIPP, uncertainty from the second concern (i.e., correlations) was generally neglected except in a few cases (e.g., permeability of halite, $k_{x,halite}$, and permeability of anhydrite, $k_{x,MB}$, in Salado in 1991 PA [13]) where it was treated by introducing rank correlations in conjunction with Latin Hypercube Sampling (LHS) [45; 63].

Uncertainty from the use of a limited number of measurements was handled by fitting available data to a "Student-t distribution" by the method of moments (i.e., calculating the sample mean, variance, and setting the degrees of freedom to the one less than number of samples). It is well known that, in a Bayesian approach, the Student-t distribution can represent the distribution of the true mean, given a sample mean formed from a small number of measurements [21, p. 80] (i.e., when data was available at WIPP, n_{sample} was typically < 10). The t distribution has slightly fatter tails than a normal distribution with a standard error of the mean of $\sigma_\varphi/\sqrt{n_{sample}}$ where σ_φ was the standard deviation of the sample for the parameter φ_n [98]. The corresponding normal distribution with a standard error of $\sigma_\varphi/\sqrt{n_{sample}}$ would have been adequate for many situations encountered in the WIPP PAs (i.e., the uncertainty in the two distributions is already similar for n_{sample} equal to 10 since a 98% confidence interval is $\mu \pm 2.82\ \sigma_\varphi/\sqrt{n_{sample}}$ for the t distribution versus a 98% confidence interval of $\mu \pm 2.33\ \sigma_\varphi/\sqrt{n_{sample}}$ for the normal distribution); however, the use of the t distribution, in addition to being more correct, alerted a reviewer that the distribution represented the uncertainty in the mean value of the parameter, not the observed local variability between various measurements.

In the 1996 PA, five sampled parameters were represented by t distributions (Fig. 7). These parameters represented material properties of the Marker Bed 139 anhydrite strata (Fig. 3) in the repository flow submodel [51], $\mathcal{R}_{BRAGFLO}(\bullet)$: permeability ($k_x$), rock bulk compressibility (β_{fB}), residual brine saturation (s_{lr}), residual gas saturation (s_{gr}), and pore-distribution exponent in the Brooks-Corey model (λ_{Brooks}). (These five parameters were 100% correlated with the five corresponding parameters in the two-anhydrite layers modeled above the repository [Fig. 3].)

Since the t distribution is infinite, the distribution should usually be truncated. However, the use of default confidence intervals for the t distribution, such as 0.01and 0.99 quantiles as used for the normal distribution above, can produce unreasonably large bounds when the number of samples is small (e.g., $\mu_k \pm 3.36\ \sigma_k / \sqrt{n_{sample}}$ for 6 samples used to determine permeability for Marker Bed 139, which produces a lower bound near the permeability of pure halite and an upper bound near the permeability of consolidated waste—Ref. [17], Figure 18). Certainly, less stringent quantiles might be used when the number of samples is small (e.g., 0.10 and 0.90 quantiles) and the quantiles increased as the number of samples increases (e.g., 0.05 and 0.95 and eventually 0.01% and 0.99). However, the reasonableness still must be evaluated. Because this evaluation is likely to be heavily based on the range of sample values collected, for the 1996 PA, the default truncation was set at the measured minimum and maximum data values used to calculate the distribution. The parameter development team then evaluated the reasonableness of the range.

6. Other Issues

6.1 Other Approaches

Both simple and complex approaches have been reported for setting parameter distributions (e.g., Refs. [16; 61; 89; 99]). A few examples are as follows.

The international study of climate change from greenhouse gases is a program that it striving to provide a large set of data that is consistently developed for use in various models. The guidance is as follows [99]:

(i) Where empirical data are available, the first choice should be to assume a normal distribution of the data (either in complete or truncated form to avoid negative value, if these would be unrealistic), unless the scatter plot of the data suggest a better fit to another distribution;

(ii) Where expert judgement is used, the distribution function should be normal or lognormal as in (i), supplemented by uniform or triangular distributions as described in Annex 3;

(iii) That other distributions are used only where there are compelling reasons, either from empirical observations or from expert judgement backed up by theoretical argument.

Several reasons possibly exist for this more simplified approach. First, the number of parameter types is much less (essentially, one: the amount of each type of greenhouse gas), thus, the participants could more readily specify a preference for the normal or lognormal PDF. Second, the models where the data would be used had not been specified at this point; thus, more processing of the data would likely be necessary to develop a model parameter that was appropriate for the intended use.

Lipton et al. proposed a two-tiered process in 1995 [89]:

(1) fitting sample data to know statistical distributions (with known properties) and

(2) using default distributions from the literature if fitting sample data is unsuccessful.

The first phase suggested by Lipton et al. involved a number of intermediate steps that included first using distributions frequently used in the literature; second, attempting to fit available data to various classes of distributions and using goodness-of-fit techniques to assess the viability; and third, using the empirical data directly in the sampling scheme when large amounts of data existed. The second phase involved using both default distributions frequently used in the literature or selecting the uniform distribution. While some similarities exist to the approach used on the WIPP, the Lipton et al. approach neglects the vexing issue of whether the empirical data available were representative at the temporal and spatial scales needed in the model.

Much earlier, the International Atomic Energy Agency (IAEA) [61; 106] specified more inclusive steps:

> Parameter uncertainty analysis should be composed of the following steps:
>
> 1. Define the assessment endpoint. This may be an annual dose to a member of a "critical group," the collective dose to a defined population, or the lifetime health risk to an average individual, a maximally exposed individual, or an unspecified individual in the population.
> 2. List all potential important uncertain parameters. Include additional parameters, if necessary, to represent uncertainty in the model structure.
> 3. Specify the maximum conceivable range of possible applicable values for uncertain parameters with respect to the endpoint of the assessment.
> 4. For this range, specify a (subjective) probability distribution that quantitatively expresses the state of knowledge about alternative values for the parameter (i.e., defines the probability that the true value of the parameter is located in various subintervals of the indicated range).
> 5. Determine and account for dependencies that are suspected to exist among parameters...

Except for the first step, the outline of steps is similar to the underlying general outline for the WIPP parameter process (the WIPP process is, however, far more detailed). For WIPP, the first step was the initial step of the overall iterations. At WIPP, the EPA selected an assessment "endpoint" in 40 CFR 191 (the normalized, cumulative release at a boundary—Eq. (1)) and the limiting criterion for this endpoint. Furthermore, the EPA specified that parameters related to the exposure pathway were to be "expected values," as already mentioned in Section 2.1. When using the WIPP process outside a PA analysis, the influence of the endpoint on parameter definition should be an additional explicit step since it could be important in some situations. For example, if the end point is the maximally exposed individual, then distributions for parameters that define the human behavior of the individual should apply to the hypothetical maximally exposed individual, not average human behavior.

6.2 Risk Dilution

Committees of the Nuclear Energy Agency (NEA) of Organisation of Economic Co-operation and Development and the IAEA [107] have coined the term "risk dilution" where "risk" is a placeholder for whatever performance measure is being used and "dilution" refers to the use of overly broad ranges for parameter distributions of the disposal system model. The situation given is where the performance measure is mean peak dose at a human receptor (the performance measure for radioactive waste disposal at Yucca Mountain in Nevada [40 CFR 197] [32; 34] and in many European countries). The concern cited is where the parameters that influence the

time of peak dose are assigned overly broad ranges such that the time of the peak dose varies greatly, and, thus, the mean peak dose averaged over numerous simulations is greatly reduced from that calculated with narrow distributions. At WIPP, "dilution" of the performance measure was not a primary concern. In 40 CFR 191 [27; 29], the EPA specifically avoided peak dose as a performance measure since at the time, the agency thought it was too easily manipulated by the assumed (a) release rate of radioisotopes from the waste, and (b) dispersion coefficients in the geologic barrier [108]. Rather, the EPA chose as a performance measure the cumulative release across a boundary over a specified period and normalized by the original radioactive waste inventory (Eq. (1)) [28]. This choice required the EPA to convert from recognized dose limits to a derived limit on the cumulative release, but the EPA thought this drawback was preferable to problems associated with using peak dose.[27] However, the use of inappropriate distributions (as "risk dilution" indirectly implies) was very much of concern at WIPP. An SME may have been over confident and specified a range too narrow (e.g., the minimum permeability of halite in the Salado in 1989 PA), and at other times, an SME may have been overly cautious and specified a range too broad (e.g., waste permeability in 1989 PA). However, a vigilant Parameter Lead in the later PAs and especially the 1996 PA helped an SME be evenhanded, declining to stretch distributions in favorable and unfavorable directions and widths if unjustified.

6.3 Sensitivity of Results to Distribution Type

The guidance in Section 3 had the parameter development team focus on the distribution range (e.g., subjective estimate, $\mu_\varphi \pm 2.33\sigma_\varphi$ for empirical data of small sample size) and the guidance in Section 4 had the team consistently select distribution types based on MEF and model scale (e.g., t distribution for empirical data collected at small scale). The WIPP Project did not specifically examine the sensitivity of the model results to changes in the form of the parameter distribution; rather, the sensitivity analysis yielded a ranking of the importance of the parameters themselves. Only in selected sensitivity studies were distribution types changed. For example, when evaluating the influence of a modified waste form on the performance of the repository distribution types and ranges were changed [17]. To reflect a modified waste form in the 1989 PA [38], the room matrix porosity (ϕ_m) was changed from a normal to a lognormal distribution (resulting in the mean decreasing by a factor of 2), the room hydraulic conductivity (and thus permeability, k_x) was decreased four orders of magnitudes, and the solubility range for all actinides (S_e) was decreased two orders of magnitude. To reflect a modified waste form in 1990 PA, the room permeability (k_x) was again decreased four orders of magnitude and porosity decreased one order of magnitude [17; 70].

In a major sensitivity evaluation to determine the value of proposed future experiments [76; 109], numerous distributions were changed to reflect SME predictions of what new experiments might reveal about the parameter range. This sensitivity analysis provided information for making management decisions and served to confirm

[27] For the proposed repository at Yucca Mountain, the US Congress required the EPA to use dose as the performance measure (Pub. L. 102-486). Two advantages are (a) to avoid concerns about the appropriateness of the derived limits to unique situations (e.g., gaseous release of ^{14}C) and (b) to be more comparable to the international community [32; 34]. A disadvantage is the already mentioned sensitivity to time factors such as release rates and dispersion coefficients that make "risk dilution" more of a concern and, possibly, demands for using very long-lived engineered containers [26; 33].

sensitivity information obtained directly from the 1991 and 1992 PAs [1]. However, the distribution range was the primary focus of the sensitivity analysis not the distribution type.

Except for these selected sensitivity studies, distribution types were not changed for two reasons. First, the primary performance measure was the *mean* of the cumulative release observed in the analysis and the mean is not often strongly influenced by the distribution type [89]. Second, and most importantly, the process of developing the distributions, described in Sections 3 and 4, sought to establish the best description of the epistemic uncertainty given the known underlying data and the use of the parameter in the model. Granted the distribution type can influence extreme quantile values [89; 110]; however, an SME typically described his degree of belief about the appropriate value of a parameter (epistemic uncertainty) using a truncated distribution with fat tails (e.g., 75% of sampled parameters in 1996 PA used uniform or histograms [Fig. 7]); thus, there was usually adequate sampling of extreme (but still physically plausible) values in the WIPP PAs.

7. Summary

The manner in which Sandia conducted the assessment of the performance of the WIPP helped generate favorable scientific and regulatory support for the repository. The consistent and traceable assignment of parameters values and distributions was an important part of this overall methodology, as summarized below.

7.1 PA Strategy

Three general points of the overall PA strategy for the WIPP were pertinent to the development of parameter distributions: detailed modeling, periodic iterations, and evaluation of reasonable expectation. The use of detailed models allowed the WIPP Project to explore many potential sources of uncertainty and tie any lack of understanding of sources of uncertainty more directly to physically meaningful and measurable data (rather than a parameter that subsumed many physical processes). An important goal of iterating the PAs was to focus resources on issues and thus models and parameters that mattered [45; 111]. The 1996 PA [8] of the WIPP was the culmination of four preliminary PAs (1989 through 1992) [38; 39; 40; 41; 42; 43]. The evaluation of reasonable expectation placed a requirement to be neither too optimistic nor too pessimistic about the uncertainty in a parameter value.

7.2 Types of Parameter Uncertainty

The evaluation of reasonable expectation required that the WIPP Project quantify uncertainties realistically and over their full range of the state of knowledge, rather than estimate conservative bounds. In this regard, the WIPP Project divided uncertainty into two classes: (1) aleatoric uncertainty about plausible scenarios (sequence of features, events, and processes) whose separate analysis was warranted because of WIPP Project or outside interest; and (2) epistemic uncertainty derived from (a) uncertainty associated with model form, and (b) uncertainty associated with model parameters. Two techniques were used to evaluate both types of uncertainty (1) *ceteris paribus* analysis by varying parameters or models (or conceivably scenarios) one at a time, and (2) probabilistic analysis when (a) the scenario probability of occurrence could be described by a probability model, (b) the selection of model form alternatives could be described by a probability model using indicial parameters, or (c) uncertainty

about the precise value of a parameter could be described with a probability distribution. The vast majority of parameter distributions defined were material-property parameters used to describe the physical or chemical properties of various materials within the modeling domain of the WIPP PA.

7.3 Parameter Lead

The proper assignment of a distribution required knowledge of (a) the use and scale of the parameter in the PA system model, and (b) the availability, type, and representativeness of the data. In the WIPP Project, the scientists and engineers who collected data (termed Subject Matter Experts or SMEs) were not the same scientists and engineers responsible for development and application of the PA (termed PA Analysts); however, agreement between these two groups was essential for regulatory review. For the 1990 PA [11; 70] and thereafter [13; 15], one key strategy for assigning parameter uncertainty realistically and consistently was to appoint a Parameter Lead. The two responsibilities of the Parameter Lead were (1) to provide guidance to the SMEs and PA Analysts so that the myriad parameter values and distributions necessary in a PA were consistently assigned evenhandedly, and (2) to ensure that reviewers could readily understand the basis for a parameter distribution. Obviously, the purpose of the analysis will determine the care necessary in assigning parameter distributions. However, at least the role and function of a Parameter Lead should be recognized for small projects when limited by resources. The position should be funded at least part time if the project is big enough for the SME and PA Analyst to be separate individuals.

7.4 Process of Assigning Distributions

The steps in the Sandia process consisted of (1) PA Analysts identifying needed parameters, (2) SMEs identifying and documenting available data (and often proposing distributions), (3) the Parameter Lead, PA Analysts, and SME meeting jointly to develop (or evaluate proposed) distributions, and continuing with additional meetings until disputes were resolved, (4) documenting the parameter distribution decision, placing the parameter in a data base, and internal review of documentation, (5) department decisions on parameters to sample in the PA and design of sensitivity analysis. The third step was the primary topic of this paper. In the third step, the team used one of three general approaches to develop a distribution: (a) direct use of data; (b) use of all available information to develop a subjective distribution [112]; and (c) following regulatory guidance or occasionally following scientific precedence in the literature.

Bayesian updating was never used in iterations of the PA because of (a) changes in the underlying data from new and newly interpreted experiments, and (b) changes in the meaning of parameters in models. Rather, the parameter development team started the process over when describing the distribution for each necessary parameter identified.

It took time to develop this three-member parameter development team. For the 1989 and 1990 PAs, the responsibility for assigning parameter values fell more heavily upon the Parameter Lead. Training of SMEs and PA Analysts occurred prior to the 1991 PA such that the PA Analysts and SMEs took on more responsibility within the team thereafter.

7.5 Selection of Distribution Types

The selection of distribution types, whether based directly or indirectly on empirical information, was developed under several guidelines: First, distributions selected usually satisfied the maximum entropy formalism. The majority of distributions in each PA were either uniform or histogram (piecewise uniform) PDFs. Generally, the WIPP Project used the uniform PDF in early iterations at WIPP followed by more detailed examination of the range and specification of the histogram (piecewise uniform) PDF for those parameters found important in sensitivity analysis, as previously noted [111]. Other distribution types used included the Student-*t* triangular, normal, and beta PDFs. Distribution types occasionally used included the discrete delta and exponential PDF.

Second, logarithmic transforms of the parameter values were used typically (but not always) whenever the ratio of the maximum and minimum of the range was greater than 100 (i.e., $b_\varphi/a_\varphi > 100$). When $10 < b_\varphi/a_\varphi < 100$, a logarithmic transform was often used but other factors were taken into account.

Acknowledgements

The responsibility of the position of the Parameter Lead and number of tasks that had to be completed grew with each iteration. Both authors wish to generally acknowledge the support many individuals provided during that time; two individuals in particular are M-A Martell, Sandia National Laboratories and HJ Iuzzolino, GRAM, Inc. The production of the final 1996 PA for the WIPP required many individuals with expertise in several areas of science and technology. This paper could not cite all the excellent and creative subject matter experts and PA Analysts, but they are gratefully acknowledged. (The special issue of *Reliability Engineering & System Safety* [8] and three references cited [1; 5; 6] provide an extensive list of contributors). The authors wish to thank S Halliday for verifying references, and F Puffer, SK Best, and DJ Rivard of Ktech Corporation, for editorial, illustration, and word processing support, respectively. The authors also wish to thank the internal reviewers at Sandia—JC Helton, M-A Martell, C Hansen, and MJ Mitchell—for their helpful suggestions to the text. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000. WIPP programs administered by the DOE funded this work.

Appendix I: Parametric Uncertainty

As previously noted, in the WIPP PA the elements of the *nP*-tuplet $\mathbf{p}$, the argument of $R(\bullet)$, was conceptually divided into three disjoint subsets [2; 54]: (1) a class of certain, fixed parameters, $\mathbf{p}^F$; (2) a class of uncertain parameters, $\mathbf{p}^A$, whose elements, for the WIPP, represented future events; and (3) a class of remaining uncertain parameters, $\mathbf{p}^E$. Various names for the second and third uncertain parameters are as follows.

The $\mathbf{p}^A$ class contains those parameters in probability models of aleatoric events. Aleatoric events are assumed to have a random character in the sense that their likelihood of taking place in various intervals of space or time can be estimated statistically, but it is not possible to determine whether or not they will actually occur. These chance events were used to form scenarios in designing the PA simulation or within a submodel $\mathfrak{R}_\alpha(\bullet)$ of $R(\bullet)$ when it was practical to evaluate the probability of a scenario with a probability model. For the WIPP this inexactness arose

because both human intrusion through exploratory drilling (or mining) and no exploratory drilling (or no mining) were possible states of the disposal system that the regulator felt needed to be explicitly analyzed.

In other analysis, aleatoric uncertainty has also been called Type 1 (e.g., Ref. [55]), Type A [35], stochastic (e.g., Refs. [54; 57]), variable uncertainty (e.g., 10 CFR 63.114, Ref. [32] and Ref [113]), or irreducible uncertainty. Both aleatoric and stochastic formally refer to randomness in processes (e.g., radioisotope decay), but the general lack of knowledge about the future state of the system (e.g., intrusion or no intrusion) is now also associated with these words. The term "variable uncertainty" emphasizes the variability among individual characteristics of a population. This type of inexactness cannot be reduced through further testing and data collection (e.g., variability in the human population or variability in geologic media cannot be reduced through further testing); it can only be better described ("characterized"), and, thus, this first type of parameter uncertainty is also referred to as irreducible uncertainty.

The parameters in class $\mathbf{p}^E$ were designated epistemically uncertain parameters. Epistemic uncertainty arises from a lack of knowledge about the value of a parameter because the data are limited or because there are alternative interpretations of the available data. An epistemically uncertain parameter is not variable because of an intrinsic characteristic of the entity but because an analyst does not know what the precise value of the parameter should be. Epistemic uncertainty is also called Type 2 (e.g., Ref. [55]), Type B, subjective (e.g., Refs. [9; 54]) state of knowledge, or reducible uncertainty. Epistemic refers to the "state of knowledge" about a parameter. The state of knowledge about the exact value of the parameter can increase through testing and data collection such that the uncertainty is "reducible." Epistemic uncertainty also includes model uncertainty (i.e., what is the appropriate model or model structure to use in a particular modeling context). For WIPP there was substantial epistemic uncertainty in many parameters (e.g., the solubility of radioisotopes in the repository environment). Further, as noted above, there can also be epistemic uncertainty in parameters used to characterize aleatory uncertainty. Conceptually, the parameter specifying the mean of the distribution of times of occurrence of the aleatoric exploratory drilling (i.e., the rate, λ_{drill}, at which human intrusions occur in a Poisson probability model), was epistemically uncertain since empirical data concerning the occurrence of the event were unknown and could only be surmised from past drilling practices.

The WIPP analysis used probability to characterize the aleatory and epistemic uncertainty; however, the interpretation of the term probability for these two types of uncertainty was different [55]. For aleatoric uncertainty, the meaning of term "probability" took the frequentist interpretation (even though sufficient data were seldom available from which to determine frequencies). For epistemic uncertainty, the term "probability" took the Bayesian interpretation (i.e., degree of belief).

Appendix II: Assigning Parameters of Numerical Models Involving Heterogeneous Media

In the United States, performance assessments of geologic waste disposal systems often entail, for the sake of realism, numerical solutions of partial differential equations (PDEs).[28] A realistic assessment of the role of the

[28] However, PDEs are often implicit in the simplified, lumped-parameter mathematical models that underlie other policy analyses, e.g. studies involving the prediction of the spread of a disease throughout the population of a heterogeneous urban area.

disposal system in preventing release of radioisotopes to the accessible environment require that PDEs governing flow and solute transport through porous/fractured geologic media be solved to yield predicted radioisotope discharge at boundaries of the disposal system specified by the environmental standards set, for example, by the EPA. Furthermore, the choice of the appropriate model parameters values and corresponding uncertainty in these values are directly tied to the choice of the conceptual model, the material zones modeled, and numerical grids used. As an example, we use the equation governing transport through saturated rock of a reactive solute species that undergoes radioactive decay [114]:

$$\nabla \bullet (\mathbf{D} \bullet \nabla C - C\nu) = \phi R \frac{\partial C}{\partial t} + \phi R C \lambda_{rad} \qquad \text{(II-1)}$$

where the two variables are the solute concentration (mass per unit volume of solvent) at point $\mathbf{x}$ within the medium[29] at time t, $C(\mathbf{x}, t)$, and the local advective velocity of the fluid in the rock pore space (usually supplied as an independent field resulting from solution of flow equations), $\nu(\mathbf{x}, t)$. The local material property parameters (i.e., characteristics of the medium sustaining the flow) for a porous media are the dispersion tensor, $\mathbf{D}(\mathbf{x})$; porosity, $\phi_m(\mathbf{x})$; the retardation factor, $R_{Kd}(\mathbf{x}) = 1 + (\rho_{bulk}(\mathbf{x})/\phi(\mathbf{x}))Kd_e(\mathbf{x})$; and the radioactive decay constant, $\lambda_{rad} = \ln(2)/t_{1/2}$ (i.e., $\mathbf{p} = \{(\mathbf{D}(\mathbf{x}), \phi_m(\mathbf{x}), \ln(2)/t_{1/2}, \rho_{bulk}(\mathbf{x}), Kd_e(\mathbf{x})\}$. The diagonal elements D_L and D_T of $\mathbf{D}(\mathbf{x})$ are a function of molecular diffusion and longitudinal and transverse dispersivity (i.e., $D_L = \phi_m(\mathbf{x})D^o_e + \alpha_L|\nu(\mathbf{x}, t)|$ and $D_T = \phi_m(\mathbf{x})D^o_e + \alpha_T|\nu(\mathbf{x}, t)|$ where $\alpha_T \cong 0.1\alpha_L$).

In geologic media, the local material properties are usually highly variable; thus, the model domain must be divided into regions were any one parameter φ in $\mathbf{p}$ can be considered constant. But even in the case when local material properties are constant over space, two- and three-dimensional versions of Eq. (II-1) seldom if ever permit a closed-form or analytic solution; invariably, recourse is made to a numerical model that attempts an approximate solution of Eq. (II-1) with its attendant specified source-terms and boundary conditions. Construction of a numerical model entails dividing the flow domain into a finite number of contiguous cells and finding finite-difference or finite-element approximations to Eq. (II-1) that can be solved on a computer in a reasonable amount of time. For a typical cell in the computational mesh of a three-dimensional flow domain, the j^{th} cell has volume V_j and six sides having areas A_{ij}, $i = 1,\ldots,6$. One way of approximating Eq. (II-1) on the domain of cells is to form the volumetric average of Eq. (II-1) over each cell. As shorthand we define volumetric (and areal) averages of each cell as [112].

$$<\varphi>_V \equiv \frac{1}{V}\iiint_V \varphi(\mathbf{x})\, dV, \quad <\varphi>_A \equiv \frac{1}{A}\iint_A \varphi(\mathbf{x})\, dA$$

where $\varphi(\mathbf{x})$ is any spatially variable parameter defined in the domain of the computational mesh. Taking the volumetric average of the j^{th} cell in Eq. (II-1) gives

[29] The solute concentration and all other quantities in Eq. (II-1) are volume averages over small "representative elementary volumes" (REVs) [Ref. 15, 112] such that the porous media can at least be considered a continuum. However, the appropriate volume for the model may need to be much larger than this minimum.

$$\sum_{i=1}^{6} \frac{A_{ij}}{V_{j-cell}} < \mathbf{F} \bullet \boldsymbol{\xi}_i >_{A_{ij}} = \frac{\partial}{\partial t} < \phi R_{Kd} C >_{V_j} + \lambda_{rad} < \phi R_{Kd} C >_{V_j} \qquad \text{(II-2)}$$

where **F** is the flux, ($\mathbf{D} \bullet \nabla C - C\boldsymbol{v}$), and $\boldsymbol{\xi}_i$ is the unit outward normal vector on surface of area A_{ij}. We have used Gauss' theorem to change the volume integral of the divergence of the flux (left side of Eq. (II-1)) into a surface integral of the normal component of **F** over the surface enclosing the j^{th} cell. If we define the effective concentration in cell j as

$$C_j(t) \equiv \frac{\langle \phi R_{Kd} C \rangle_{V_j}}{\langle \phi R_{Kd} \rangle_{V_j}},$$

then, after some rearrangement of terms, Eq. (II-2) can be written as an ordinary differential equation (ODE) for effective concentration in the j^{th} cell:

$$\frac{dC_j}{dt} = -\lambda_{rad} C_j + \frac{1}{\langle \phi R_{Kd} \rangle_{V_j}} \sum_{i=1}^{6} \frac{A_{ij}}{V_{j-cell}} < \mathbf{F} \bullet \boldsymbol{\xi}_i >_{A_{ij}} . \qquad \text{(II-3)}$$

By extension, similar equations can be written for other cells in the computational mesh, leading to a system of ODEs. Although software exists for efficient numerical solution of large systems of ODEs, numerical schemes for solving PDEs usually replace the time derivatives of the dependent variables by finite-difference approximations, making both time and spatial domains discrete. The equations for the effective concentrations $C_k(t)$, $k = 1,2,\ldots,j,\ldots$, are coupled via difference approximations to gradients and cell-surface quantities appearing in **F**. It is seen that the parameters of a numerical model such as Eq. (II-3), i.e. the various volumetric and areal averages, are different from those appearing in the PDEs from which the numerical model is derived. In particular, parameters of numerical models involving heterogeneous, imprecisely characterized geologic media are not directly measurable because the volume average of a parameter in a numerical model is not the same and often much bigger than the measurement scale of the data (even though we might use the same word, such as porosity or permeability, to describe both entities). Thus, professional judgment is necessary to develop the distribution, not just statistical analysis of the experimental data,

The foregoing description of a process for going from a PDE to a system of equations that can be numerically solved is intended to aid further discussion of the following issue: How does one use laboratory or field measurements of the rock material properties appearing in Eq. (II-1) to assign physically realistic values to the parameters in a numerical model such as Eq. (II-3)?

Most physical and chemical properties of geologic or engineered materials at WIPP were measured on spatial scales typical of the laboratory or an exploratory borehole, a matter of tens of centimeters at most. Yet, for the solution of the numerical model to remain tractable in the WIPP numerical analysis, elements and cells had to have dimensions of tens of meters near the repository and hundreds of meters far away and corresponding volumes in the thousands to millions of cubic meters. The fact that the parameters in computational model solving the mathematical model specified in Eq. (II-3) are represented as volume or areal averages of representative element volume scale quantities suggests that we treat the experimental values as samples at selected points of random fields

[115] and the model parameters as spatial averages of those random fields. The connection between spatial averages and ensemble averages of random fields can be illustrated by an example.

Assume that a material-property parameter, $\varphi(\mathbf{x})$, can be represented as a scalar random field (The assumption of a scalar quantity is for the sake of simplicity of the following argument and involves no loss of generality; the property could be a vector or tensor.) More precisely, assume that $\varphi(\mathbf{x})$ is a locally stationary, random scalar field within a computational cell of volume $V_{j\text{-}cell}$ with the following statistical properties [116]:

Expectation of $\varphi(\mathbf{x})$ within cell = $\mathcal{E}[\varphi_{cell}] = \mu_{\varphi,cell}$, a constant, and

Covariance of $\varphi(\mathbf{x})$ within cell = $\mathcal{E}[(\varphi_{cell}(\mathbf{x}) - \mu_{\varphi,cell})(\varphi_{cell}(\mathbf{y}) - \mu_{\varphi,cell})] = \sigma^2_{\varphi,cell}\, \psi(|\mathbf{x}-\mathbf{y}|)$

where $\sigma^2_{\varphi,cell}$ is the variance of φ within the cell and $\psi(\bullet)$ is the autocorrelation function that measures the statistical dependence of the values of $\varphi(\bullet)$ at two different points $\mathbf{x}$ and $\mathbf{y}$. Although $\mu_{\varphi,cell}$ and $\sigma^2_{\varphi,cell}$ are assumed constant within a cell, they may vary between cells. The autocorrelation function, $\psi_\varphi(\bullet)$, has the properties: $\psi_\varphi(r) \geq 0$ for $r \in (0,\infty)$; $\psi(r) \to 1$ as $r \to 0$; $\psi(r) \to 0$ as $r \to \infty$. Under these conditions, it can be shown that

$$\text{Expectation of } \langle \varphi_{cell} \rangle_V \text{ or } \langle \varphi_{cell} \rangle_A = \mu_{\varphi,cell} \tag{II-4}$$

$$\text{Covariance of } \langle \varphi_{cell} \rangle_V \text{ or } \langle \varphi_{cell} \rangle_A = \frac{\sigma^2_{\varphi,cell}}{V^2_{j-cell}} \int_V \int_V \psi_\varphi(|\mathbf{x}-\mathbf{y}|)\, d\mathbf{x}d\mathbf{y} \tag{II-5}$$

If μ_φ, σ_φ^2, and $\psi_\varphi(\bullet)$ were known, the problem could be solved in that the distribution of the material property parameters, $\langle \varphi(\mathbf{x}) \rangle_V$ or $\langle \varphi_n \rangle_A$, could be approximated by a normal distribution with mean and variance as given above. Conceivably, μ_φ, σ_φ^2, and $\psi_\varphi(\bullet)$ could be estimated from spatially coordinated measurements of the local material property $\varphi(\mathbf{x})$ (i.e., $\varphi(\mathbf{x}_1)$, $\varphi(\mathbf{x}_2)$,...$\varphi(\mathbf{x}_n)$). Yet, there were few spatially coordinated measurements available at WIPP. Only four parameters ($\mathbf{p} = \{\mathfrak{I}_K, \rho_{grain}, \phi_m, \tau_{tort}\}$) of the Culebra were spatially indexed at wells and of these only $\mathfrak{I}_K$ was treated as a field parameter.

Inferences about the appropriate values of all other material-property parameters used in WIPP computational models eventually were based on the following two observations. First, the variance of a material property parameter in any cell or element of the large-scale, numerical PA model is less than or equal to the apparent variance of the material property at the local scale (i.e., because $\psi(\bullet) < 1$, then the integrand of Eq. (II-5) is always less than one so that variance of a cell or $\sigma^2_{cell} \leq \sigma^2_{local}$. In particular, if the form of the autocorrelation function is taken as a "cookie cutter" (i.e., $\psi_\varphi(|\mathbf{x}-\mathbf{y}|) = 1$ if $|\mathbf{x}-\mathbf{y}| \leq r$, otherwise $\psi_\varphi(|\mathbf{x}-\mathbf{y}|) = 0$) then

$$\sigma^2_{cell} \cong (V_{local}/V_{j\text{-}cell})\sigma^2_{local}$$

where $V_{j\text{-}cell}$ is the volume of the j^{th} numerical cell or element over which the physical quantity is to be averaged and V_{local} is the volume of correlation, $(4/3)\pi r^3$. Although the volume of correlation is not precisely known, it is often known that $V_{local} << V_{j\text{-}cell}$ and consequently the variance of the spatially averaged parameter is so much smaller than the variance of the parameter on a local scale that it can be neglected. In which case, the only uncertainty is that associated with μ_φ as discussed below.

Second, if as argued in Eq. (II-4) above, $\langle \varphi_{cell} \rangle_V$ or $\langle \varphi_{cell} \rangle_A \cong \mu_\varphi$, then one must estimate the uncertainty inherent in estimating μ_φ that may arise from (1) the correlation that may occur between μ_φ and other uncertain

parameters of the PA model, and (2) a finite number of measurements (i.e., $\varphi(\mathbf{x}_1)$, $\varphi(\mathbf{x}_2)$,...$\varphi(\mathbf{x}_n)$) of the material property at the scale of an representative element volume. Concerning the first item, uncertainty from correlation was generally neglected except in a few cases in each PA. Concerning the second item, the Central Limit Theorem ensures that the uncertainty in the true mean is normally distributed with a mean standard error (σ_{MSE}) of $\sigma_{local}/\sqrt{n_{sample}}$ when numerous but still a finite number of measurements are available. As an example, the local matrix porosity of the Culebra (ϕ_m) from 20 boreholes varies between 0.096 and 0.250 with $\sigma_{local} \cong 0.04$ and $\sigma_{local}/\mu_\phi = 0.27$ (Ref. [70], p. 2-84). Based on the Central Limit Theorem, the uncertainty in the mean porosity of 0.15 is quite small ($\sigma_{MSE} \cong 0.009$ and $\sigma_{MSE}/\mu_\phi = 0.06$). Because of the small coefficient of variation for the mean porosity ($\sigma_{MSE}/\mu_\phi < 0.08$), Culebra matrix porosity was not sampled in the WIPP PAs. However, note that the use of the local-scale spatial variability in porosity (σ_{local}) to estimate the parameter uncertainty would result in a standard deviation for the uncertainty distribution that was a factor of $\sqrt{20}$ larger than the standard error and might well prompt one to sample porosity. The consequences of using the spatial variability on a local scale instead of uncertainty in the mean volume average would be, in a Monte Carlo sampling scheme, the frequent selection of unphysically large or small mean values and the possible distortion of sensitivity analyses (i.e., inflated importance of parameters which are actually insensitive).

Although numerous measurements were available for matrix porosity (79 measurements in the 20 boreholes), the number of local measurements available (n_{sample}) was typically < 10 in WIPP experiments. For the situation of a limited number of measurements, the uncertainty in the true mean is described by a Student-*t* distribution[30] with the same mean standard error (σ_{MSE}).

Although the question of scale is a common example of when a parameter in an equation is not the same as measured data, other examples include the situation where one parameter lumps together several concepts. An example is $Kd_e(\mathbf{x})$ *in* the expression for the retardation factor in Eq. (II-1) (i.e., $R_{Kd}(\mathbf{x}) = 1 + (\rho_{bulk}(\mathbf{x})/\phi(\mathbf{x}))Kd_e(\mathbf{x})$). The representativeness of experimental conditions for evaluating $Kd_e(\mathbf{x})$ for future repository conditions can be questioned. Hence, while scaling is an uncertainty issue for $Kd_e(\mathbf{x})$, uncertainty concerning the time varying water chemistry, time varying chemical species in solution, and systematic changes in mineralogy of the Culebra must also be lumped into the uncertainty distribution for the $Kd_e(\mathbf{x})$ parameter as well.

[30] In a Beyesian sense, the normal and *t* distribution are conjugate pairs.

Appendix III: Proof Histogram PDF (Piecewise Linear CDF) Maximizes Entropy

The central problem of the maximum entropy formalism is the determination of extrema of the entropy functional $U(g)$ defined by

$$U(g) = -\int_a^b g(\varphi)\, ln(g(\varphi))\, d\varphi$$

over the set of all probability density functions (PDFs) for the parameter φ ($g(\varphi)$) that are nonzero in the range $[a, b]$ and which satisfy prescribed constraints best expressed as integral constraints, i.e. constraints taking the form

$$\int_a^b z_m(\varphi)\, g(\varphi) d\varphi = c_m,$$

where $m = 0, 1, \ldots, nM$ and the z_m are functions integrable over the closed interval $[a, b]$. One necessary constraint on a PDF is that its integral over $[a, b]$ must equal one; thus, one conventionally sets $z_o(\varphi) = 1$ and $c_0 = 1$. By expressing the constraints in this way, one can derive a general solution to the problem (in the calculus of variations) of maximizing $U(g)$ subject to $nM+1$ constraints [19]. The maximizing PDF, here denoted by $g^*(\varphi)$, is given by

$$g^*(\varphi) = Z^{-1}(\gamma)\exp[-\sum_{m-1}^{nM} \lambda_m z_m(\varphi)],$$

where $\boldsymbol{\gamma}$ denotes the vector $(\gamma_1, \gamma_2, \ldots, \gamma_{nM})$ and Z^{-1} is the reciprocal of Z given by

$$Z(\boldsymbol{\gamma}) = \int_a^b \exp[-\sum_{m-1}^{nM} \gamma_m z_m(\varphi)]\, d\varphi\,.$$

The γ_m, $1 \le m \le nM$, are Lagrange multipliers (constants) to be determined by solving the following set of nM equations in nM unknowns:

$$-(\partial/\partial\gamma_m) ln Z(\boldsymbol{\gamma}) = c_m,\ m = 1, 2, \ldots, nM.$$

Let the empirical or subjective quantile points of a CDF be given as $nM \ge 1$ ordered pairs $(\varphi_1, \wp_1)$, $(\varphi_2, \wp_2)$, $\ldots$, $(\varphi_{nM}, \wp_{nM})$ in the closed interval $[a, b]$ where $0 \le a < \varphi_1 < \ldots < \varphi_{nM} \le b < \infty$ and $0 < \wp_1 < \wp_2 < \ldots < \wp_M < 1$. For convenience, define $\varphi_o = a$, $\wp_o = 0$, $\varphi_{nM+1} = b$ and $\wp_{nM+1} = 1$. The maximum entropy constraints on the candidate PDF, $g(\varphi)$, may then be written as

$$\int_a^b H(\varphi_m - s) g(s) ds = \wp_m,$$

where m is 0, 1, $\ldots$, $nM+1$ and $H(\bullet)$ is the Heaviside unit step function [117, p. 1020]. With these constraints, the PDF, $g(\varphi)$, that maximizes the entropy functional $U(g)$ is found to be

$$g^*(\varphi) = \exp\left[\sum_{m-1}^{nM} \gamma_m H(\varphi_m - \varphi) - 1\right]$$

where

$$Z(\boldsymbol{\gamma}) = \int_a^b \exp\left[-\sum_{m-1}^{nM} \gamma_m \delta(\varphi_m) d\varphi\right] = 1$$

where $\delta(\bullet)$ is the Dirac-delta function. Inspection of $g^*(\varphi)$ shows that it is a piecewise-constant function on the closed interval $[a, b]$; i.e., $g^*(\varphi) = q_m$ *for* $\varphi_{m-1} < \varphi \le \varphi_m$ with Q_m a different constant for each $m = 1, 2, \ldots, nM$. The constants q_m are related to the constants γ_m, and it is easier to determine q_m from the constraints. For example, consider the integral of $g^*(\varphi)$ between φ_{m-1} and φ_m:

$$\int_{\varphi_{m-1}}^{\varphi_m} g^*(\varphi)\, d\varphi = q_m(\varphi_m - \varphi_{m-1})$$

from the constraints, the integral is also equal to

$$\int_{\varphi_{m-1}}^{\varphi_m} g^*(\varphi) d\varphi = \wp_m - \wp_{m-1}$$

Hence,

$$q_m = (\wp_m - \wp_{m-1}) / (\varphi_m - \varphi_{m-1}) \text{ for } m = 1, 2, \ldots, nM+1.$$

The CDF associated with the PDF, $g^*(\varphi)$, is found by integrating $g^*(\varphi) = q_m$ between a and point $\varphi > a$, yielding the piecewise-linear CDF:

$$G^*(\vartheta) = \begin{cases} 0, & \text{if } 0 < \vartheta \le a \\ \wp_{m-1} + (\wp_m - \wp_{m-1})(\vartheta - \varphi_{m-1})/(\varphi_m - \varphi_{m-1}), & \text{if } \varphi_{m-1} < \vartheta \le \varphi_m \\ 1, & \text{if } \vartheta > b \end{cases}$$

We do not know whether this piecewise uniform PDF is an unbiased estimator of the unknown distribution $G(\vartheta)$ when the assigned percentiles and percentile points represent empirical measurements of the random variable underlying the distribution. However, the discrete delta PDF (piecewise uniform CDF) is an unbiased estimator [96, 214-216]. The question of unbiased estimators is of course meaningless when the assigned quantiles are subjective estimates by SMEs.

Appendix IV: Parameter symbols

$A_{i,j}$	Surface area of side *i of* j^{th} numerical grid cell
a_φ	Minimum of distribution range
b_φ	Maximum of distribution range
$C(\mathbf{x}, t)$	Dissolved concentration of actinide (mass per unit volume of solvent) at point **x** within the medium at time t ($C_{b,El(l)}$ —Ref. [52]; C_k—Ref. [53])
D^o_e	Molecular diffusion of element e in pure fluid (m^2-s) (D^*_k—Ref. [53]; *MD0*—Ref. [71], App. A)
$\mathcal{D}_n$	Element domain space of **R** consisting of a set of model parameters (**p**), spatial variables (**x**), and time (t)
$\mathbf{D}(\mathbf{x})$	Diagonal dispersion tensor with elements D_L, D_T, and D_T where $D_L = \phi_m(\mathbf{x})D^o_e + \alpha_L \lvert v(\mathbf{x}, t)\rvert$ and $D_T = \phi_m(\mathbf{x})D^o_e + \alpha_T \lvert v(\mathbf{x}, t)\rvert$ ($\mathbf{D}_k$—Ref. [53])
d_{drill}	Drill bit diameter of intrusion borehole (m) ($2R_\sigma$—Ref. [80]; *DIAMMOD*—Ref. [71], App. A))
$\mathfrak{E}[\bullet]$	Expectation operator; for example, $\mathfrak{E}[\varphi_n]$ is $\int \varphi_n\, g_\alpha(\varphi_n)\, d\varphi_n$, which is the mean of parameter φ_n (i.e., μ_φ)
$\mathbf{F}$	mass flux and equal to $\mathbf{D}(\mathbf{x})\nabla C(\mathbf{x}, t) - C(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)$
$\mathcal{F}_{Brooks}$	Flag to select Brook-Corey, Van Genuchten-Parker, or linear model formulae for P_{cap}, k_{rw}, k_{rg} for anhydrite MB (*ANHBCVGP*—Ref. [9], Table 1; Ref. [51], Table 4;*RELP_MOD*—Ref. [71], App. A)
$f_{mine\text{-}trans}$	Mining transmissivity multiplier ($f_{mine\text{-}trans}v(\mathbf{x})$–Ref. [53]) (*MINP_FAC*—Ref. [71], App. A)
$\mathcal{G}_\alpha(\varphi_n)$	Cumulative distribution function (CDF) of parameter φ_n where α identifies distribution type (e.g., α = *uniform*)
$g_\alpha(\varphi_n)$	Probability density function (PDF) of parameter φ_n
g_{grav}	Acceleration due to gravity, physical constant (m/s^2) (*GRAVACC*—Ref. [71], App. A)
$H(\bullet)$	Heaviside unit step function; $H(t - T) = 0$ if $t \le T$ and 1 if $t > T$
$H_{freshH2O\text{-}well}$	Measured freshwater head at 41 wells in Culebra (m) (i.e., $H_{freshH2O} = f(\mathbf{x})$)
Kd_e	Adsorption partition coefficient (m^3/kg) for element e = Am^{III},Pu^{III},Pu^{IV},Th^{IV},U^{IV},U^{VI} (K_{dk} —Ref. [53]; *CMKDAM3*, etc. —Ref. [9], Table I; e.g., *MKD_AM*—Ref. [71], App. A)
K_H	Hydraulic conductivity, $f(\mathbf{x})$ in Culebra ($K_H(\mathbf{x}) = k_\mathbf{x}\rho_{fluid}g_{grav}/\mu_{fluid}$) (**K**—Ref. [53])
k_x, k_y, k_z	Intrinsic permeability of various materials in x, y, or z direction defining diagonal elements of **k** tensor (m^2) ($f(t)$ for consolidating salt) ($k_\mathbf{x} = 10^{mat}$ where *mat* = e.g., *ANHPRM, BHPRM, BPPRM, HALPRM, SHPRMASP*, —Ref. [9], Table 1;e.g., *APORO, PRMX_LOG*—Ref. [71], App. A)
n_{sample}	Number of samples
$\wp\{\bullet\}$	Probability model; for example, $\wp\{S_j\}$ is probability of scenario class S_j
$\wp_n$	Discrete probability value associated with a discrete value of parameter φ_n
${}^{max}\wp_\varphi$	Mode of $g_\alpha(\varphi)$ where α is usually *triangular*.
$\mathbf{P}$	Ordered nP-tuplet set of individual parameters (φ_n); three major subsets include certain, epistemic uncertain ($\mathbf{p}^E$), and aleatoric uncertain ($\mathbf{p}^A$).
$R_{Kd}(\mathbf{x})$	Retardation of dissolved radioisotope species $(1 + (\rho_{bulk}(\mathbf{x})(1\text{-}\phi(\mathbf{x})Kd(\mathbf{x}))$ (R_k—Ref. [53])

$\mathbf{R}(\bullet)$	WIPP total disposal system or consequence model that functionally transforms the element domain space ($\mathcal{D}_n$) into the results range space
$\mathcal{R}_\alpha(\bullet)$	Submodel α of the WIPP total disposal system model, $\mathbf{R}(\bullet)$ (e.g., α = *BRAGFLO* or *PANEL* in Fig. 3)
R	Radial distance
$r_{type\text{-}shaft}$	Shaft radius where *type* = air (3.09 m), exhaust (2.3 m), salt (1.8 m), or waste (3.5 m), or DRZ (e.g., *RSH_AIR* or *RADN_DRZ*—Ref. [71], App. A)
S_j	Scenario class *j*
S_e	Logarithm of dissolved solubility limit for element *e* (S_D(Br,Ox,El) dissolved solubility for brine type Br, oxidation state Ox, and element El —Ref. [52], Table 1; *LOGSOLM*—Ref. [71], App. A)
s_{gr}, s_{lr}	Residual saturation (gas phase, liquid brine phase) (Ref. [51]; e.g., *ANRGSSAT*, *SHRGSSAT*, *WRGSSAT*,—Ref. [9], Table 1; e.g., *SAT_RGAS*—Ref. [71], App. A)
$\mathcal{T}_K$	Transmissivity (m^2/s) $\mathcal{T}_K = \boldsymbol{K}_H(\mathbf{x})\Delta z(\mathbf{x})$ (T(x,y) —Ref. [53])
$T_{1/2\text{-}I}$	Half-life of radioisotope *i* (s) (*HALFLIFE*—Ref. [71], App. A)
t	Time
$U(\varphi_n)$	Informational entropy of parameter $(-\sum \varphi_n \ln \varphi_n)$
$V_{j\text{-}cell}$	Volume of j^{th} numerical grid cell
V_{local}	Volume of geologic medium over which parameter is correlated
$\nu(\mathbf{x}, t)$	Fluid velocity as function of $\mathbf{x}$ and *t* (m/s) (**v**—Ref. [53]; $\mathbf{v}_b$—Ref. [52])
$\mathbf{x},\mathbf{y}$	Spatial location (*x, y, z)* vectors (m)
α_L, α_T	Dispersivity, either longitudinal or transverse; used to determine diagonal elements of dispersion tensor, $\mathbf{D}(\mathbf{x})$ ($\alpha_T \cong 0.1\alpha_L$) (m) ($\alpha_L$—Ref. [53]; e.g., *DISPL_L*—Ref. [71], App. A)
β_{fB}	Bulk compressibility of solid (Pa^{-1}) (e.g., *ANHCOMP*, *HALCOMP*—Ref. [9], Table 1; Ref. [51]; *COMP_RCK*—Ref. [71], App. A)
γ_m	Lagrange multipliers, $1 \le m \le Nm$
$\delta(\bullet)$	Dirac delta function; $\delta(t - T) = 1$ if $t = T$ and zero if $t < T$ or $t > T$
λ_{Brooks}	Brooks-Corey pore-distribution parameter exponent (λ—Ref. [51]; e.g., *AHNBCEXP*, *SHCEXP*—Ref. [9], Table 1; *PORE_DIS*—Ref. [71], App. A)
λ_{drill}	Drilling rate for Poisson probability model of human intrusion via exploratory drilling (λ_d—Ref. [57]; *LAMBDAD*—Ref. [71], App. A)
λ_{rad}	Radioactive decay rate ($\ln(2)/t_{1/2}$) (s^{-1}) (λ_I—Ref. [52]; λ_k—Ref. [53])
μ_φ or $\mu(\varphi_n)$	Mean of parameter φ_n
μ_{fluid}	Viscosity of *fluid* = mud, gas-mud mixture, Castile brine, Salado brine (Pa-s or kg/m-s) (μ_b—Ref. [51]; η—Ref. [80]; *VISCO*—Ref. [71], App. A)
ξ_i	Unit outward normal vector on surface of area A_{ij} ($\mathbf{n}$(x,y)—Ref. [52])
π	Mathematical constant (*PI*—Ref. [71], App. A)
$\rho_{solid\text{-}material}$	Density (*solid* = bulk or grain) of *material* =Fe-CH,Fe-CHdrum,paper-CH (kg/m^3) (e.g., ρ_s—Ref. [53]; e.g., *DIRONCHW*—Ref. [71], App. A)
ρ_{fluid}	Density of *fluid* = Salado brine, Castile brine, mud ($kg\text{-}m^3$) (ρ_b—Ref. [51]) (*DNSFLUID*—Ref. [71], App. A)

σ_φ or $\sigma(\varphi_n)$	Standard deviation of parameter φ_n
$\tau_{tort\text{-}material}$	Tortuosity $(l\text{-}l_{path})^2$ of *material* = clay, dolomite (τ—Ref. [53]; *TORTUSTY*—Ref. [71], App. A)
τ_{fail}	Shear strength of waste (Pa) (τ_{fail}— Ref. [80]; (*WTAUFAIL*—Ref [9], Table 1)
ϕ_m	Matrix diffusive porosity (e.g., *CMTRXPOR, HALPOR*—Ref. [9], Table 1; *POROSITY*—Ref. [71], App. A)
$^{50\%}\varphi_n$	Median value of $g(\varphi_n)$
φ_n	Individual parameter of $\mathbf{R}(\bullet)$
$\psi(\bullet)$	Autocorrelation function that measures the statistical dependence of the values of φ at two different points **x** and **y**

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